

*Prepared for:*

**SETTLING DEFENDANTS**

**Revision 1**

**CO-LOCATION OF DIOXINS/FURANS  
AND AROCLOR 1268**

**LCP CHEMICALS SITE  
OPERABLE UNIT 1  
BRUNSWICK, GEORGIA**

*Prepared by:*



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February 2019

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A handwritten signature in black ink, appearing to read "Kirk Kessler".

Kirk Kessler, P.G.  
Senior Principal

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# 1 INTRODUCTION

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## 1.1 Background and Executive Summary

This co-location study was performed in accordance with Appendix B of the Consent Decree between Honeywell and the Georgia Power Company (“GPC”) with the United States Environmental Protection Agency (“USEPA”), *The United States v. Honeywell International Inc. et al.*, Civil Action No. 2:16-cv-00112, which was filed in the United States District Court for the Southern District of Georgia, with an effective date of July 27, 2017 (“Consent Decree”). Collectively, Honeywell and GPC are herein referred to as the Settling Defendants (“SDs”). The Consent Decree addresses the salt marsh that constitutes Operable Unit 1 (“OU1”) of the LCP Chemicals Superfund Site in Brunswick, Georgia (“Site”).

USEPA examined past sampling for PCDD/Fs at the Site and local area in a memorandum as part of the Record of Decision (“ROD”) for OU1 (USEPA, 2014, 2015). The memorandum provided an evaluation on the association (*i.e.*, co-location) of polychlorinated dibenzodioxins/furans (“PCDD/F”) in OU1 sediments with Aroclor 1268, presenting evidence that a high degree of co-location exists. Due to the somewhat limited PCDD/F data set used in the 2014 evaluation, USEPA concluded in the memorandum that “additional [PCDD/F] sampling will be required to confirm the dioxin furans conceptual site model, *i.e.*, that Aroclor 1268 and dioxin furans are co-located and that remediating the former will reduce dioxin furans concentrations to acceptable levels.”

The present study conducted in 2018 involved strategic sampling targeting the various portions of OU1 designated for Remedial Action, contributing numerous additional characterization points in OU1 to supplement prior OU1 sampling for paired Aroclor 1268 and PCDD/F testing. In doing so and based on the collaborating results of the 2018 co-location study, the Conceptual Site Model (“CSM”) developed in 2014 by the USEPA is further validated.

The statistical evaluation provides clear and meaningful evidence of the strong association of PCDD/F with Aroclor 1268 in the OU1 sediments. This allows the following factors to support the conclusions developed from the Aroclor 1268 characterization in OU1, to be applied to PCDD/F, and no further assessment is necessary. In summary:

1. The paired test results support the CSM regarding co-location, and thus remediating the PCB condition will remediate a similar PCDD/F condition.
2. The highest PCDD/F condition occurs in the portion of Eastern Creek beyond the area of the past Removal Action dredging, where the highest condition in Eastern Creek should be expected (according to the CSM).

It is well documented that the tidal channel sediments exhibit a significantly higher contaminant condition relative to the adjoining marsh flats. Remediating the full extent of Eastern Creek in the OU1 Remedial Action will address the elevated dioxin toxic equivalency (“TEQ”) present in that channel.

## 1.2 Terms of Reference

According to 3.1(f)(1) of Appendix B (Statement of Work) of the Consent Decree: “[The Pre-Design Study (PDS)] includes verification sampling to confirm that polychlorinated dibenzodioxins/polychlorinated dibenzofurans (“PCDD/Fs”) and Aroclor 1268 are co-located.” (USEPA, 2016). The study design was provided in the *Co-location Study Work Plan* (Appendix B to the *Remedial Design Work Plan*) dated March 28, 2018 and approved by the USEPA on April 16, 2018.

## 2 CONCEPTUAL SITE MODEL – ASSOCIATION OF PCDD/F WITH AROCLOR 1268

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### 2.1 Site Setting

The Site occupies approximately 880 acres immediately northwest of the City of Brunswick, Glynn County, Georgia (Figure 1) and is comprised of approximately 760 acres of salt marsh and 120 acres of high ground (uplands). The upland area, where manufacturing operations at the Site occurred, is bordered by the Glynn County Detention Center and Public Works to the north, Ross Road to the east, and Brunswick Cellulose to the south.

### 2.2 OU1 Features

The LCP marsh is characterized by vegetated marsh flats dissected by numerous channels and larger creeks under tidal influence from Turtle River. These features provide a physical segregation of OU1 into “domains”, as illustrated on Figure 2. The principal feature of the marsh is Purvis Creek, which enters the marsh on the Site from the Turtle River at the southwest corner and ends at the northeast upland-marsh border. Smaller tidal channels and creeks existing in the LCP marsh include the Main Canal, Eastern Creek, Western Creek Complex, Landfill Creek, and Domain 3 Creek (Figure 2).

### 2.3 Release of Aroclor 1268 and PCDD/F Compounds to OU1

From 1913 to the mid-1970s, chlor-alkali processes commonly used graphite blocks as anodes in the electrolysis process (O’Brien *et al.*, 2005). The graphite anodes contained coal tar pitch as a bonding agent, and cyclic aromatic compounds (such as dibenzofuran) were common constituents of the coal tar pitch. Successive chlorination of cyclic aromatic compounds present in the coal tar has been proposed as the primary mechanism for formation of PCDFs during the chlor-alkali process (consistent with the findings of Yamamoto *et al.*, 2017).

Graphite block anodes were used at the Site until the mid-1970s. Furthermore, Aroclor 1268 which is a form of polychlorinated biphenyls (“PCBs”), was impregnated into the graphite anodes for a period of time in the 1960s to condition the anode block prior to placement in the electrolytic cell. Thus, Aroclor 1268 was also characteristic of the graphite sludge at the Site.

The facility also generated process wastewater, which prior to the enactment of the Clean Water Act in 1972, was discharged with little treatment to the marsh (Domain 1). During the ebb tide cycle, these waters would follow the Main Canal to Purvis Creek. During the flood tide cycle, water flow reversed “upstream” serving to push the diluted wastewater stream into Eastern Creek

and into the upper reaches of Purvis Creek (Figure 3). At the approximate middle portion of the flood tide, the water level overtops the banks of the tidal channels flooding the marsh flats, spreading to the point of the “tidal node” where it meets flood tide waters from an adjacent channel. During high tide, suspended contaminated particles could be transported over the banks into the marsh. However, once out of the channel, the rapid increase in cross-sectional area and resistance to flow caused by the marsh grasses lowers water velocities and limits the transport distance of particulate-bound chemicals into the marsh (ENVIRON and Anchor QEA, 2013).

## 2.4 Physical-Chemical Properties

PCBs such as Aroclor 1268, and PCDD/Fs are nonpolar compounds and are characterized as hydrophobic. With a  $\log K_{ow} > 7.4$ , Aroclor 1268 partitions strongly to non-polar substances (e.g., organic matter). PCDD/Fs exhibit similar behavior (tetrachlorinated PCDD compounds have a  $\log K_{ow} > 6.8$ ). Because of the strong hydrophobic composition of Aroclor 1268 and PCDD/Fs, adsorption to organic (primarily) and inorganic particles defines the fate and transport of these compounds in the estuarine environment.

Sediment transport and sedimentation are the dominant processes that determine the fate of PCBs in OU1 (Black & Veatch, 2011). Because Aroclor 1268 and PCDD/Fs exhibit similar physical-chemical properties and were released to the marsh associated with the same source, PCDD/Fs are expected to adhere to the same fate and transport processes as Aroclor 1268 and be co-located with Aroclor 1268.

## 2.5 Distribution of Aroclor 1268 and PCDD/F in OU1 Sediments

The distribution of Aroclor 1268 and PCDD/F in the OU1 sediments is consistent with the CSM presented in the preceding sections. Figure 4 shows the original Aroclor 1268 concentration distribution from sediment sampling conducted across OU1 prior to the 1998-99 removal response action. The Aroclor 1268 distribution shows the highest condition bordering the Domain 1 shoreline and upper reach of the Main Canal. A high degree of spatial attenuation is expressed east to west across the Domain 1 marsh flats, and to the south along the shoreline owing to the dense vegetation of the marsh flats. A more moderate degree of spatial attenuation is expressed in the tidal channels, whether in the Main Canal (east to west) or in Eastern Creek (north to south). A similar distribution pattern is exhibited for the pre-removal PCDD/F condition, expressed as the dioxin TEQ value<sup>1</sup> (Figure 5). Table 1a provides a summary of paired PCDD/F congeners and Aroclor 1268 historical sampling results.

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<sup>1</sup> PCDD/F congener data are commonly evaluated as a single result, where each congener concentration is normalized to the congener 2,3,7,8-TCDD using congener-specific toxicity equivalency factors (“TEFs”) (van den Berg *et al.*, 2006) and the values are summed to generate a PCDD/F TEQ value. The present TEF scheme is based on 2005 values reported by the World Health Organization.

## 2.5.1 PCDD/F Homologue Profiles

### 2.5.1.1 Overview

A simple histogram graphical representation of the 10 PCDD/F homologue classes can be used to illustrate the “chemical fingerprint” or profile of the PCDD/F condition. This method of data analysis can be used to identify commonality (or lack thereof) of the source of PCDD/F to individual sample sites from the study area. PCDD/F congener profiling of historical sediment samples collected in the vicinity of the Site and in the regional vicinity of Brunswick, Georgia reveal two distinct PCDD/F congener patterns: (i) a PCDF-dominant profile consistent with byproducts of the chlor-alkali process (Kannan *et al.*, 1997; Rappe *et al.*, 1991; and Yamamoto *et al.*, 2017<sup>2</sup>), and (ii) a PCDD-dominant profile associated with the regional condition.

PCDD/F profiles were created from the five PCDD and five PCDF congener groups (see table below) as a compositional percentage of the total congeners concentration for a given sample.

Dioxin Congeners	Total HpCDDs	Total HxCDDs	OCDD	Total PeCDDs	Total TCDDs
Furan Congeners	Total HpCDFs	Total HxCDFs	OCDF	Total PeCDFs	Total TCDFs

Profiles characterized from upland soils, Turtle River/regional sediments, and LCP marsh sediments are discussed in the following sections. Table 1b provides the PCDD/F homologue results from these prior sampling events.

### 2.5.1.2 Upland Profile

Two soil samples from Sprenger *et al.* (1997) and one soil sample from Kannan *et al.* (1997) capture the upland soil condition prior to the 1995-1997 upland removal action. These samples exhibit a strong PCDF signature (as shown in Chart 1 below) consistent with the historical byproducts of the chlor-alkali process and may be used for comparison with patterns measured in OU1 sediment samples.

<sup>2</sup> In the Yamanoto *et al.* study, exclusively PCDD/Fs were formed in tests using graphite electrodes.

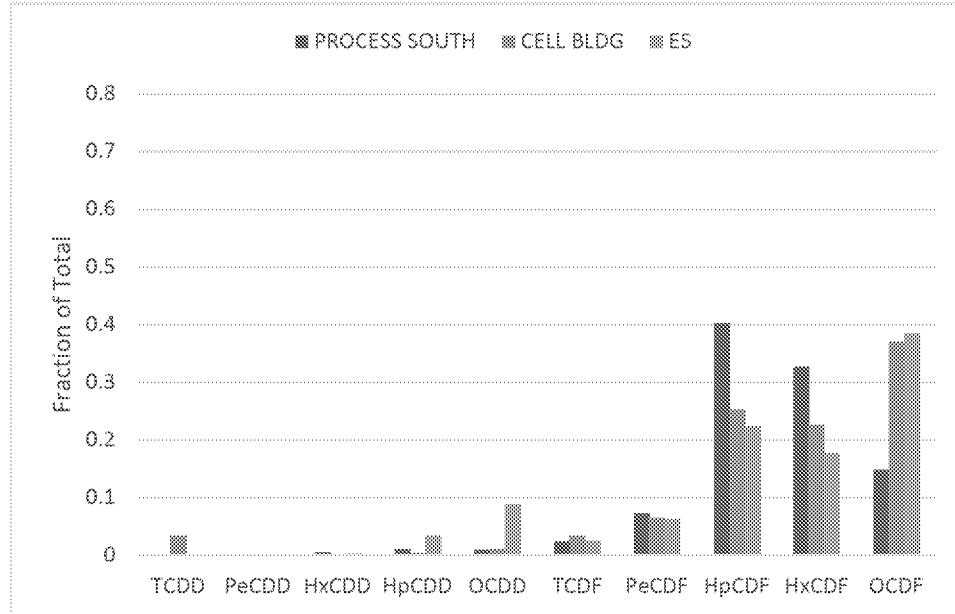


Chart 1. PCDD/F homologue profiles for upland soil samples

### 2.5.1.3 Turtle River/Regional Profile

A regional-based study known as the “Brunswick Initiative”, a collaborative effort involving USEPA and the Georgia Environmental Protection Division (“EPD”), included collection and testing of sediment samples within the Turtle River Estuary, St. Simons Sounds, and areas east of the Brunswick Peninsula. The homologue patterns reveal a PCDD-dominated profile comprised mostly of OCDD followed by HpCDD and HxCDD homologue groups.

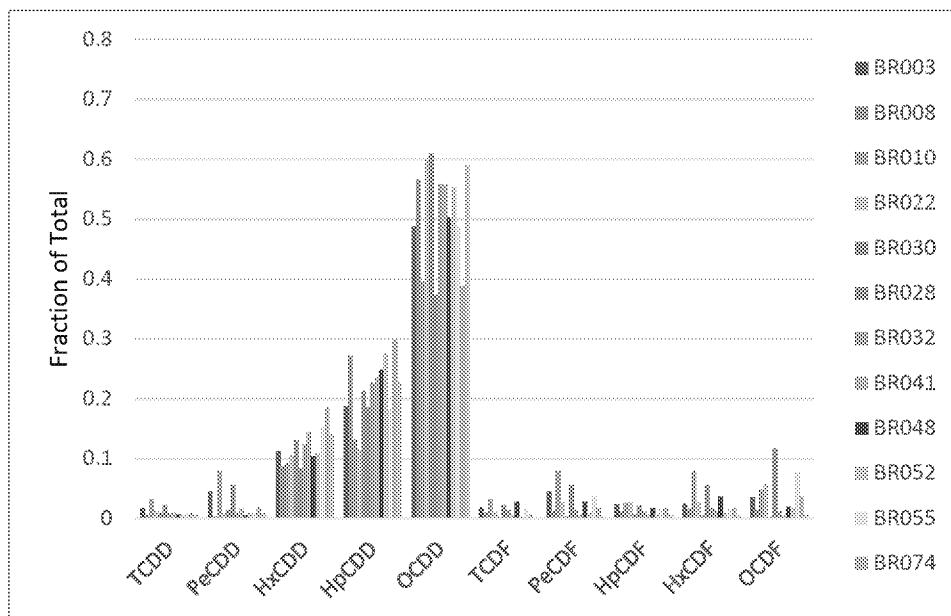


Chart 2. PCDD/F homologe profiles for samples collected during Brunswick Initiative Study

#### 2.5.1.4 LCP Marsh (OU1)

Sediment samples collected by USEPA from 1995-1996 and CDR and Geosyntec (2001) characterize the condition in OU1. Homologue profiles for these samples are provided below (Charts 3 and 4). Profiles for samples collected proximate to the Outfall Pond former discharge point exhibit a strong PCDF pattern mixed with similar concentration of OCDD and HpCDD homologue groups, suggesting a mixed environment of Site-related and regional influences. Further afield in OU1 (Purvis Creek and Western Creek Complex sample locations), the pattern shifts further to a dominant PCDD profile similar to the regional condition. The shift from the PCDF to PCDD profile along the concentration gradient suggests that Site influence diminishes to the regional condition further into OU1. Figure 6 illustrates the spatial relationship of the past PCDD/F sampling results in terms of the homologue profile pattern shift from the uplands (source) across OU1 (mixed environment).

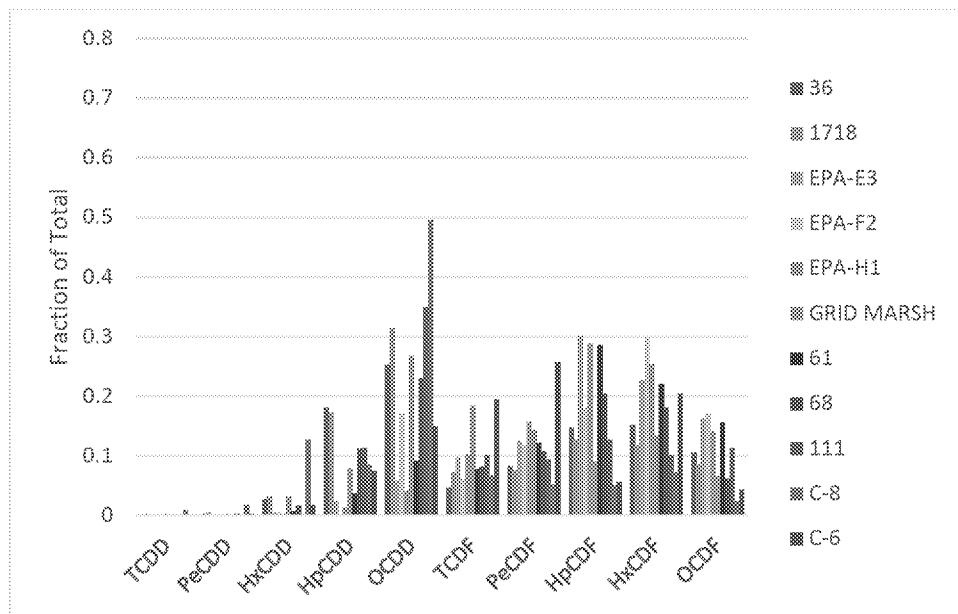


Chart 3. PCDD/F homologue profiles for Domain 1 and associated tidal channels (Eastern Creek and Main Canal).

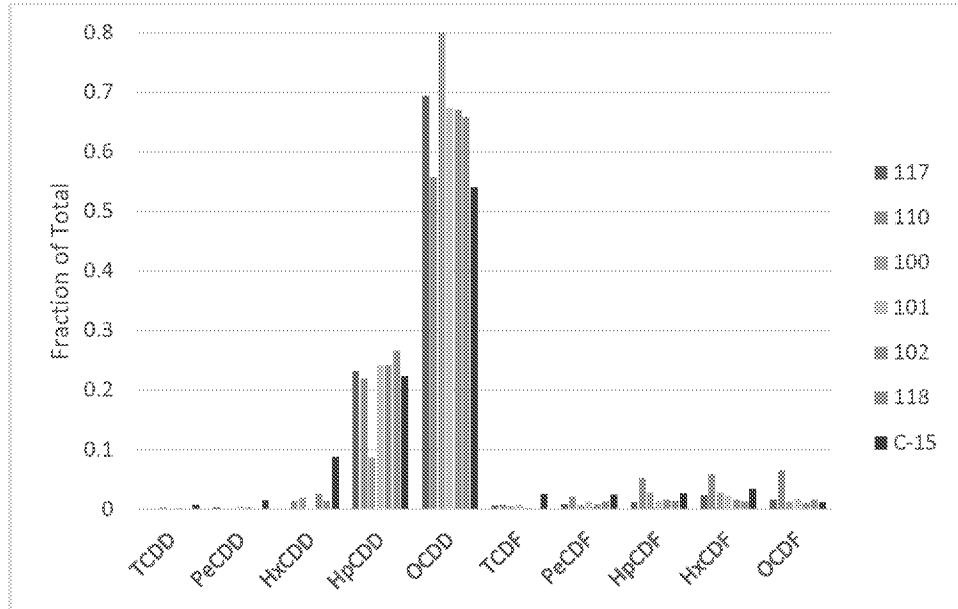


Chart 4. PCDD/F homologue profiles for samples collected from Purvis Creek and Western Creek Complex.

## 2.6 1998-99 OU1 Removal Action

From 1998 to 1999, approximately 13 acres of marsh flats in the near-shore area of Domain 1 were excavated, backfilled, and revegetated with indigenous marsh grasses (Figure 7). Dredging was also performed in a portion of Eastern Creek and the Main Canal. Some of the current co-location sampling was performed in the removal action areas, and it should be expected that dioxin congener profiles (and TEQ concentration) have been altered in comparison to the pre-removal condition representations presented in prior sections of this report. These elements are considered in the data evaluation section presented later in this report.

### 3 SAMPLING LOCATIONS FOR CO-LOCATION STUDY SUPPORT

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Surficial sediment (*i.e.*, upper 6 inches) sampling for the co-location study was performed at 14 areas, 28 total locations, in accordance with the EPA-approved Work Plan. Sampling areas targeted the planned OU1 Remedial Action areas, with a greater sampling density toward historical sediment sampling locations that exhibited a more dominant PCDF congener profile indicative of a greater level of Site-related contribution. Sampling locations are summarized below and illustrated on Figure 8:

- Thin-layer cover Remedial Action areas (south of the causeway)
  - one sampling area on the marsh flats flanking the causeway at the upper end of the Main Canal (D1-1)
  - one sampling area on the marsh flats between the 13-acre removal action area and Eastern Creek (D1-2)
  - one sampling area at the south end of Eastern Creek on the marsh flats to the west (D2-1)
- Dredging Remedial Action areas
  - three sampling areas within the Main Canal (MC-1, MC-2, MC-3)
    - of these, areas MC-1 and MC-2 are in areas of the former Removal Action dredging
  - four sampling areas within Eastern Creek (EC-1, EC-2, EC-3, EC-4)
    - of these, areas EC-1 and EC-2 are in areas of the former Removal Action dredging, area EC-3 at the approximate terminating point of that dredging, and area EC-4 beyond the former dredging limits
- Capping Remedial Action areas
  - one sampling area in each of three portions of Purvis Creek designated for remedial action (PC-1, PC-2, PC-3)
  - one sampling area in Domain 3 Creek<sup>3</sup> (LC-1).

Each sampling area consisted of two adjacent, 5-foot by 5-foot sub-areas, resulting in two independent samples at each sampling area (*e.g.*, D1-1A and D1-1B for area D1-1). Each sample was collected as a composite of sediment (from 5 points<sup>4</sup>) within each sub-area from a depth interval of approximately 0-6 inches. The sample units that make up each composite were homogenized in a stainless-steel bowl prior to transfer to the sampling container. Sediments from marsh flats were collected using a stainless-steel spoon. Sediments from Purvis Creek and smaller tidal channels of the LCP marsh were collected using a hand auger. Clean (decontaminated)

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<sup>3</sup> This portion of the Domain 3 Creek feature has been referred to as “Landfill Creek” in some of the past documents.

<sup>4</sup> At times additional sub-sampling points were necessary, owing to hard substrate and minimal sample recovery.

sampling equipment was used to collect each sample (*i.e.*, two sets of clean sampling equipment were used per sampling area).

All samples were labeled, placed on ice in a cooler, and logged under standard chain of custody. Sediment samples for PCB Aroclor characterization were shipped to Alpha Analytical Services in Mansfield, Massachusetts and analyzed by SW-846 Method 8082A. Sediment samples for PCDD/F characterization were shipped to SGS AXYS Analytical Services, Inc. in Sidney, British Columbia and analyzed by SW-846 Method 8290A.

# 4 RESULTS

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## 4.1 Paired Aroclor 1268 and Dioxin TEQ Results

Aroclor 1268 concentrations in sediment are mapped in Figure 9<sup>5</sup>. Concentrations ranged from 0.604 milligrams per kilogram<sup>6</sup> (“mg/kg”) (PC-3B) to 31.1 mg/kg (PC-1A) with the highest results occurring in the southern-most locations in Eastern Creek (EC-3A, EC-3B, EC-4A) and Purvis Creek north of the causeway (PC-1A, PC-1B). Dioxin TEQs in sediment ranged from 6.88 nanograms per kilogram<sup>7</sup> (“ng/kg”) (PC-3B) to 863 ng/kg (EC-3B).

Figure 9 also posts the PCDD and PCDF results in terms of the mass concentration, as well as the total dioxin TEQ (a representation of relative toxicity, not concentration). PCDD/F mass distribution exhibits a similar spatial profile to Aroclor 1268 with the highest concentration occurring at the southern-most locations in Eastern Creek (EC-3A, EC-3B, EC-4A, EC-4B), and Purvis Creek north of the causeway (PC-1A, PC-1B), as shown on Figure 9.

The spatial distributions of Aroclor 1268 and PCDD/F validate the CSM. Both constituents exhibit moderate concentration in the Domain 1 areas where previous Removal Response dredging had occurred, and more elevated concentration in the Domain 1 areas further afield in the upper reaches of Eastern Creek where past dredging has not taken place (*i.e.*, the original condition remains).

Table 2a provides the summary of PCDD/F congener and Aroclor 1268 sampling results. Appendix A provides the complete laboratory reports for the co-location study.

## 4.2 Dioxin TEQ Relative to Preliminary Remedial Goal

The ROD presented a preliminary remedial goal (“PRG”) for dioxin TEQ at 260 ng/kg, stating this as a “conservative-based remedial goal”. Sampling results are therefore compared herein to this PRG value. Sampling sites exceeding the PRG are as follows:

Location	Dioxin TEQ (ppt)	Aroclor 1268 (ppm)
PC-1A	381	31.1
PC-1B	121	24.5
EC-3A	135	24.4
EC-3B	863	22.1
EC-4A	736	28.8
EC-4B	124	7.7

<sup>5</sup> Sediment from two sample locations contained additional PCBs. Sample D1-2A reported Aroclor 1016 at 0.06 mg/kg, Aroclor 1232 at 0.09 mg/kg, and Aroclor 1260 at 0.93 mg/kg in addition to Aroclor 1268 at 1.37 mg/kg. Sample EC-1A reported Aroclor 1242 at 0.25 mg/kg in addition to Aroclor 1268 at 12.6 mg/kg.

<sup>6</sup> Also known as parts per million (“ppm”).

<sup>7</sup> Also known as parts per trillion (“ppt”).

## 4.3 PCDD/F Congener Profiles

PCDD/F homologue profile pie charts for the co-location samples are shown in Figure 10. Similar PCDD-dominant profile patterns are exhibited across the Main Canal, Domain 1 and 2 marsh flats, and proximate Purvis Creek locations – the PCDF composition at these locations comprises generally 0.1 (10%) of the total PCDD/F composition. OCDD is the predominant homologue group detected comprising about 0.5 (50%) of the total PCDD/F composition. A stronger PCDF profile (comprising approximately 0.3-0.4 (30-40%) of the total PCDD/F composition, is exhibited at the upper reach of Eastern Creek, which is consistent with the CSM as this area is beyond the limits of the past dredging conducted at the Site and retains the original chlor-alkali influenced signature.

Table 2b is a summary of PCDD/F homologue results.

# 5 STATISTICAL EVALUATION

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## 5.1 Co-location Evaluation Methods

### 5.1.1 Regression Analysis

#### 5.1.1.1 Interpretation of the Regression Analysis

An ordinary least-squares (“OLS”) regression analysis estimates a linear model that predicts the dependent variable value as a function of a single independent variable. Three key outputs of the regression analysis are the slope, coefficient of determination, and calculated probability, which are summarized as follows:

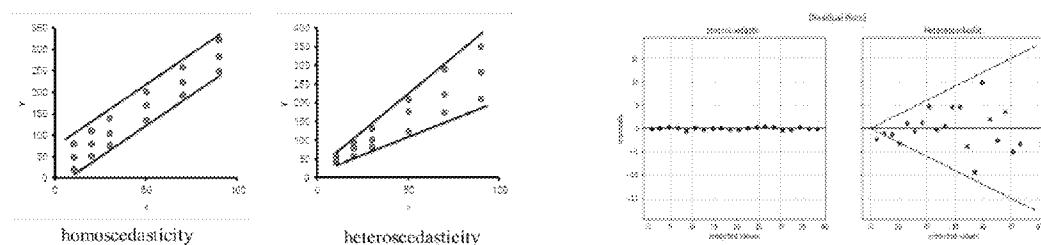
- **Slope.** The slope of the regression line ( $m$ ) represents the rate of change in the dependent variable as the independent variable changes. A slope greater than 0 indicates a positive correlation (*i.e.*, both variables move in tandem). Conversely, a slope less than 0 indicates a negative correlation (*i.e.*, one variable increases as the other decreases). A slope of 0 indicates no correlation.
- **Coefficient of Determination.** The coefficient of determination ( $R^2$ ) measures the variation in the dependent variable data explained by the model (*i.e.*, how well the linear regression fits the data set).  $R^2$  ranges from 0 to 1 where 0 indicates that the model explains none of the variability and 1 indicates that the model explains all the variability.
- **Calculated Probability.** The calculated probability (p-value) provides insight into whether the mathematical relationship derived for the sample data potentially exists in the larger population. The calculated probability tests the null hypothesis that the independent variable is not correlated with the dependent variable. If the calculated probability is less than the significance level (typically set at 5% or 0.05), the sample data provide sufficient evidence to reject the null hypothesis for the entire population.

#### 5.1.1.2 General Assumptions of Regression Analysis

According to the Gauss-Markov theorem, the OLS estimates are each a “best linear unbiased estimate” (*i.e.*, are unbiased and have the least amount of variance) of the respective population parameters when the general assumptions described below hold true. Calculations and visual aids (charts) for testing select assumptions are provided in Appendix B.

- **Zero Conditional Mean of Errors.** The unconditional mean of the population values of the random error term equals zero, *i.e.*, the residual error around the regression line is expected to be zero given any values of the independent variable. This assumption is examined by a plot of the residuals versus the independent variable (Aroclor-1268 concentration). If the residual errors are uncorrelated with Aroclor-1268 concentration, then the assumption is satisfied. All cases of co-location evaluated in Section 5.2 meet this condition (see Appendix B).

- **Independence of Errors.** The distribution of errors is random and not influenced by or correlated to the errors in prior observations. This assumption holds true for singular and pooled cross-sectional data sets (*i.e.*, random sampling performed for one event or multiple events at different points in time), such as the data evaluated in this study, as statistical independence of sample observations is implied.
- **Homoscedasticity of Errors.** Variance around the regression line is constant for all values of the independent variable (shown below). Conversely, heteroscedasticity is present when the magnitude of error differs across values of the independent variable.



Homoscedasticity in a linear regression model can be tested using the Breusch-Pagan (“BP”) Test, which calculates outputs of the OLS analysis (slope, coefficient of determination, and p-value) from an auxiliary regression of the squared residuals ( $\hat{u}^2$ ) on the independent variables. If the test statistic has a p-value below an appropriate threshold ( $p<0.05$ ) then the null hypothesis of homoscedasticity is rejected, and heteroscedasticity is assumed. White’s Test for homoscedasticity was also utilized in this analysis to confirm the results of the BP Test. White’s test relaxes the assumption of normality (Baum, 2006) and allows the independent variable to have a nonlinear effect on the error variance. The calculation is performed similar to the BP method, with outputs of the OLS analysis calculated from an auxiliary univariate quadratic polynomial of the squared residuals on the independent variables ( $\hat{Y}^2$ ,  $\hat{Y}$ ). Similar to the BP Test, if the test statistic has a p-value below an appropriate threshold ( $p<0.05$ ) then the null hypothesis of homoscedasticity is rejected, and heteroscedasticity is assumed. Calculations testing the presence of homoscedasticity for each case of co-location evaluation are included in Appendix B.

The presence of heteroscedasticity in a data set causes bias in the estimates of variance of the coefficients, and thus increases the probability of making a Type I or Type II error in hypothesis testing. In the context of this study, the regression may indicate PCDD/F is correlated with Aroclor 1268 concentration when it is in fact not (Type I error) or may incorrectly indicate that PCDD/F is not correlated with Aroclor 1268 concentration (Type II error). It is important to note that only severe heteroscedasticity may jeopardize the conclusions of the hypothesis testing. As common rule of thumb, a ratio of the generalized least square (*e.g.*, weighted least squares (see Section 5.1.1.3)) and OLS error variance<sup>8</sup> exceeding 10 indicates “severe heteroscedasticity” (Fox, 1997). Additionally, regression analysis using heteroscedastic data will still provide an unbiased estimate for the relationship between the predictor variable and the outcome (Kleinbaum, 1998).

<sup>8</sup> The higher of the two values acts as the numerator.

Data points with large residuals (outliers) and/or high leverage (*i.e.*, extreme/outlying values of the independent variable) (see Section 5.1.1.4 on Cook's Distance analysis) were removed to mitigate heteroscedasticity and justify the conclusions from hypothesis testing for the raw linear regression. Data transformation was considered as a method to mitigate heteroscedasticity; however, data transformations fundamentally transform the nature of the variable to which they are applied and may not address the hypothesis of interest regarding the original data (Feng et al. 2014; Osborne, 2002). Consequently, data transformations were not utilized in the regression analysis.

- **Normality of Errors.** The assumption of normality of errors is not necessary in linear regression analysis of sufficiently large sample size (Schmidt and Finan, 2018; Lumley et al, 2002) due to the central limit theorem, which implies that the sampling distribution of the coefficients will approach a normal distribution as sample size grows larger. A minimum sample size “sufficiently large” is commonly considered to be from greater than 10 (Schmidt and Finan, 2018) to greater than 20 (Stevens, 2009) times the number of observed parameters, or conservatively 20 samples for a simple linear regression. All cases of co-location (including those that exclude outliers) exceed a sample count of 20, thus the assumption of normality is not necessary for the regression analysis.

### 5.1.1.3 Weighted Least Squares Analysis

The method of weighted least squares (“WLS”) is an extension of OLS regression that minimizes the sum of weighted squared residuals to produce homoscedasticity. Weights that provide the expected and desired statistical properties require *a priori* information regarding the parameters (Tellinghuisen, 1996); however, it is common practice to calculate weights as the reciprocal of a squared predictor based on an auxiliary regression of the absolute value of the residuals on the independent variables. WLS regression was performed by using the “Real Statistics” (Excel Add-In) WLS data analysis tool.

### 5.1.1.4 Cook's Distance Analysis

Cook's Distance analysis estimates the influence of data point on the fitted response values of the linear regression and is useful for identifying outliers and/or high leverage points. Cook's Distance for an observation is calculated using the following equation:

$$D_i = \frac{\hat{u}_i^2}{p \text{ MSE}} \left( \frac{h_{ii}}{(1 - h_{ii})^2} \right)$$

where MSE is the mean squared error, p is the number of coefficients in the regression model,  $\hat{u}_i$  is the *i*th residual, and  $h_{ii}$  is the *i*th leverage value.

Observations scoring a Cook's Distance value above  $4/n$  (where n is the number of observations in the data set) were considered outliers and/or exert high leverage (Bollen and Jackman, 1990; van der Meeer anvd Pelzer, 2010). It is important to note that these observations are not necessarily erroneous, and therefore should not be discarded on the basis of an outlier test (EPA, 1992). Accordingly, linear regression and statistical measures of association (discussed in Section 5.1.2) were performed for each case of co-location including and excluding outlier observations, and the results were assessed collectively.

See Appendix C for Cook's Distance calculations.

### 5.1.2 Statistical Measures of Association

Statistical measures of association define the strength of the relationship or level of association between two variables in terms of the degree of monotonicity (*i.e.*, entirely increasing or decreasing). This is measured by the coefficient of correlation (R) where:

- R of +1 indicates a perfect monotonically increasing relationship;
- R of -1 indicates a perfect monotonically decreasing relationship; and
- R of 0 indicates that the relationship is not monotonic.

An R approaching +1 (monotonically increasing relationship) or -1 (monotonically decreasing relationship) indicates strong association between variables, whereas an R approaching 0 indicates weak association between variables. In the context of co-location, an R approaching +1 specifies strong association between Aroclor 1268 and PCDD/F where samples characterized by elevated Aroclor 1268 are expected to also exhibit elevated concentrations of PCDD/F and thus, suggests a high degree of co-location. The measures of association considered for evaluation of co-location are described below:

- Pearson Correlation - A parametric measure of linear correlation between two variables. Pearson's correlation coefficient ( $r_p$ ) is calculated using the following formula:

$$r_p = \frac{n(\sum x_i y_i) - \sum x_i \sum y_i}{\sqrt{(n \sum x_i^2 - (\sum x_i)^2)(n \sum y_i^2 - (\sum y_i)^2)}}$$

where  $x_i$  and  $y_i$  are the Aroclor 1268 concentration and PCDD/F ~~TEQ~~ for sediment sample  $i$  and  $n$  is the number of samples.

General assumptions of the Pearson Correlation include linearity and normality of the independent and dependent variable. If these assumptions are not satisfied, it is appropriate to apply a log-transformation to both variables to achieve linearity and normality (Bishara and Hittner, 2012; Rasmussen and Dunlap, 1991).

- Spearman Rank-order Correlation- A nonparametric measure of statistical dependence between rankings of two variables. The Spearman Correlation does not assume variables approximate linearity or normal distribution. Spearman's rank coefficient ( $r_s$ ) is calculated using the following formula:

$$r_s = 1 - \frac{6 \sum d_i^2}{n(n^2 - 1)}$$

where  $d_i$  is the difference in rank between Aroclor 1268 concentration and mass concentration of PCDD/F for sediment sample  $i$  compared to the entire data set and  $n$  is the number of samples.

## 5.2 Results of the Co-location Analysis

### 5.2.1 Overview

Co-location of PCDD/F and Aroclor 1268 were evaluated for three cases:

- Case 1 provides an evaluation on co-location of PCDD/F and Aroclor 1268 using exclusively the current 2018 co-location study sampling data set;
- Case 2 provides an evaluation on co-location of PCDD/F and Aroclor 1268 based on the combined historical and current data set for OU1; and
- Case 3 examines the paired PCDD/F and Aroclor 1268 condition in a data set comprised locations not altered by the past Removal Action – thus, the 2018 sampling locations in the Main Canal (MC-1, -2, -3) and lower portion of Eastern Creek (EC-1, -2) were intentionally excluded (this data set, therefore, offers the most representative degree of co-location).

Each case is divided into two parts (an “a” and “b”):

- The ‘a’ cases provide an assessment of the total PCDD/F mass to Aroclor 1268;
- The ‘b’ cases provide an assessment of exclusively the PCDF congener mass (believed to be more associated with the chlor-alkali production) to Aroclor 1268.

See Appendix D for complete details regarding the statistical analyses.

### 5.2.2 Case 1: 2018 Data Set

The results of the statistical analyses for Case 1 are summarized in the table below.

		Case 1a	Case 1a, excl. outliers	Case 1b	Case 1b, excl. outliers
Linear Regression	Homoscedastic	O	X	O	O
	m	721	583	402	295
	R <sup>2</sup>	0.58	0.62	0.55	0.62
	p	2.3E-06	5.4E-06	6.0E-06	5.7E-06
Pearson Correlation Analysis	r <sub>p</sub>	0.66 <sup>(1)</sup>	N/A	0.74 <sup>(1)</sup>	0.63 <sup>(1)</sup>
Spearman Rank-order Correlation Analysis	r <sub>s</sub>	0.60	0.57	0.73	0.59
	n	28	24	28	24

Notes: 'X' Denotes homoscedasticity of the data set

'N/A' denotes Pearson Correlation not applicable, data sets not normally or lognormally distributed

(1) Denotes log-transformation applied to both variables to satisfy assumptions of Pearson Correlation

O Denotes that heteroscedasticity is not severe based on ratio of WLS and OLS variance

The data set indicates co-location of total PCDD/F with Aroclor 1268. The linear regression analysis for Case 1a is statistically significant ( $p < 0.05$ ), providing sufficient evidence to reject the null hypothesis that total PCDD/F is not correlated with Aroclor 1268. The linear regression

analysis shows a positive correlation that explains 58% (including outlier observations) or 62% (excluding outlier observations) of the variation in the total PCDD/F. The Pearson correlation coefficient and Spearman rank-order coefficients for Case 1a indicate moderate increasing monotonicity (association).

Likewise, the data set demonstrates co-location of exclusively PCDF congener mass with Aroclor-1268 (Figure 11). The linear regression analysis for Case 1b indicates sufficient evidence to reject the null hypothesis that furan homologues are not correlated with the Aroclor 1268 ( $p < 0.05$ ). The linear regression shows a positive correlation that explains 55% (including outlier observations) and 62% (including outlier observations) of the variation in total furan congener mass. The Pearson correlation coefficients and Spearman rank-order coefficients for Case 1b indicate strong increasing monotonicity (association).

### 5.2.3 Case 2: Combined Historical and Current Data Sets

The results of the statistical analyses for Case 2a and 2b are summarized in the table below.

		Case 2a	Case 2a, excl. outliers	Case 2b	Case 2b, excl. outliers
Linear Regression	Homoscedastic	O	X	O	X
	m	97.5	90.4	92.1	79.7
	R <sup>2</sup>	0.87	0.80	0.87	0.86
	p	6.1E-21	2.6E-16	5.8E-21	1.9E-19
Pearson Correlation Analysis	r <sub>p</sub>	N/A	0.75 <sup>(1)</sup>	N/A	0.79 <sup>(1)</sup>
Spearman Rank-order Correlation Analysis	r <sub>s</sub>	0.71	0.66	0.80	0.77
	n	46	44	46	44

Notes:

'X' Denotes homoscedasticity of the data set

'N/A' denotes Pearson Correlation not applicable, data sets not normally or lognormally distributed

(1) Denotes log-transformation applied to both variables to satisfy assumptions of Pearson Correlation

O' Denotes that heteroscedasticity is not severe based on ratio of WLS and OLS variance

The addition of the historical samples to the current data set caused the Pearson correlation coefficients and Spearman rank-order coefficients to increase (approach +1), indicating a higher degree of co-location from Case 1 to 2. In addition, the regression analysis for Cases 2a and 2b exhibits greater statistical significance than that of their Case 1 counterpart. The regression analysis yields similar results for Cases 2a and 2b: a positive correlation expressed as a linear function that explains above 80% of the variation in the dependent variable (total PCDD/F in Case 2a and total furan homologues in Case 2b).

### 5.2.4 Case 3: Unaltered (Outside of 1998-99 Removal Action) Areas of OU1

The results of the statistical analyses for Cases 3a and 3b are summarized in the table below.

		Case 3a	Case 3a, excl. outliers	Case 3b	Case 3b, excl. outliers
Linear Regression	Homoscedastic	O	X	O	X
	m	97.2	89.2	91.8	78.5
	R <sup>2</sup>	0.86	0.80	0.87	0.86
	p	5.9E-15	1.4E-11	5.8E-15	8.6E-14
Pearson Correlation Analysis	r <sub>p</sub>	0.85 <sup>(1)</sup>	0.78 <sup>(1)</sup>	0.87 <sup>(1)</sup>	0.82 <sup>(1)</sup>
Spearman Rank-order Correlation Analysis	r <sub>s</sub>	0.78	0.74	0.83	0.79
	n	33	31	33	31

Notes: 'X' Denotes homoscedasticity of the data set

'N/A' denotes Pearson Correlation not applicable, data sets not normally or lognormally distributed

(1) Denotes log-transformation applied to both variables to satisfy assumptions of Pearson Correlation

O' Denotes that heteroscedasticity is not severe based on ratio of WLS and OLS variance

The data set indicates a high degree of co-location of total PCDD/F with Aroclor 1268. The linear regression analysis for Case 3a is statistically significant ( $p < 0.05$ ) providing sufficient evidence to reject the null hypothesis that total PCDD/F is not correlated with Aroclor 1268 concentration. The linear regression analysis shows a positive correlation that explains 86% (including outlier observations) or 80% (excluding outlier observations) of the variation in the total PCDD/F. The Pearson correlation coefficient and Spearman rank-order coefficient for Case 3a indicate strong increasing monotonicity (association), higher than other cases previously considered.

Likewise, the data set demonstrates a high degree of furan congener mass co-location with Aroclor 1268. The regressions analysis for Case 3b shows a positive correlation and provides sufficient evidence to reject the null hypothesis that furan homologues are not correlated with the Aroclor 1268 ( $p < 0.05$ ). The linear regression explains approximately 86% of the variation in total furan homologues. The Pearson correlation coefficients and Spearman rank-order coefficients for Case 3b indicate strong increasing monotonicity (association).

### 5.3 95% UCL of PCDD/F TEQ

The upper 95% confidence level on the mean concentration ("95% UCL") was computed for PCDD/F TEQ from the co-location study data set as a mode of comparison to the PRG presented in the ROD. The 95% UCL is customary to comparing results to a risk-based criterion. The 95% UCL was calculated using the EPA's ProUCL software (version 5.1). ProUCL input and output is presented in Appendix E. The 95% UCL for PCDD/F TEQ in sediment is 200 ng/kg, which is below the PRG of 260 ng/kg.

## 6 SUMMARY AND CONCLUSION

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The 2018 study involved strategic sampling targeting the various portions of OU1 designated for Remedial Action, contributing numerous additional characterization points in OU1 to supplement prior OU1 sampling for paired Aroclor 1268 and PCDD/F testing. In doing so and based on the collaborating results of the 2018 co-location study, the CSM developed in 2014 by the USEPA is further validated.

The statistical evaluation provides clear and meaningful evidence of the strong association of PCDD/F with Aroclor 1268 in the OU1 sediments. This allows the following factors to support the conclusions developed from the Aroclor 1268 characterization in OU1, to be applied to PCDD/F, and no further assessment is necessary.

1. The paired test results support the CSM regarding co-location, and thus remediating the PCB condition will remediate a similar PCDD/F condition.
2. The highest PCDD/F condition occurs in the portion of Eastern Creek beyond the area of the past Removal Action dredging, where the highest condition in Eastern Creek should be expected (according to the CSM).
3. It is well documented that the tidal channel sediments exhibit a significantly higher contaminant condition relative to the adjoining marsh flats. Remediation of the full extent of Eastern Creek in the OU1 Remedial Action will address the elevated dioxin TEQ present in that channel.

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## TABLES

Table 1a. Historical Sampling PCDD/F Congeners and Aroclor 1268 Results

	OCDD (ng/kg)	1234678HpCDD (ng/kg)	123478HxCDD (ng/kg)	123678HxCDD (ng/kg)	123789HxCDD (ng/kg)	12378PeCDD (ng/kg)	2378TCDD (ng/kg)					
TEF	0.0003	0.01	0.1	0.1	0.1	1	1					
1718	5770	798	41.4	13.4	30.1	4.9	7.8					
36	6850	1130	12.8	92.7	49.8	4.9	15.9					
61	13100	2140	42.6	57.3	38.9	8.6	29.3					
68	14800	2140	24.3	48.7	48.2	7.7	20.6					
100	1700	170	1.2	0.75	0.90	0.55	0.38					
101	1387	125	2.3	1.4	1.7	0.97	0.77					
102	1795	176	0.827	5.7	9.9	0.50	0.21					
110	690	66	0.46	0.3	0.3	0.44	0.17					
111	3286	357	11.7	7.4	8.5	3.6	1.45					
117	1481	137.8	2.6	1.65	1.913	1.5	0.78					
118	1803	184.2	2.8	1.8	2.1	2.3	1.47					
BR048	1500	190.0	3.1	8.1	11	6	4.0					
C-15	5860	610	34.2	24.4	43.0	7.2	5.7					
C-6	8810	891	11.4	24.2	40.9	6.2	53.7					
C-8	5280	597	5.0	320.0	53.0	8.70	13.4					
EPA-E3	14000	2410	48.8	52.5	50.6	12.2	14.6					
EPA-F2	20700	2420	49	503.0	192.0	15.5	1.0					
EPA-H1	22000	3480	61.1	91.6	54.4	15.40	7.3					
GRID MARSH	1600	170	4.0	8.9	8.2	0.8	7.4					
BR003	65	10	6.0	6.0	6.0	6.0	2.5					
BR008	1500	160	2.2	5.1	7.0	1.5	4.0					
BR010	30	6	6.0	6.0	6.0	6.0	2.5					
BR022	130	10	6.0	6.0	6.0	6.0	2.5					
BR028	40	6	6.0	6.0	6.0	6.0	2.5					
BR030	2600	250	5.2	9.2	19.0	3.3	1.1					
BR032	2700	310	5.1	11.0	20.0	2.9	3.8					
BR041	1700	190	4.1	7.7	15.0	2.4	1.1					
BR052	380	20	6.0	1.8	3.6	6.0	2.5					
BR055	80	10	6.0	6.0	6.0	6.0	2.5					
BR074	130	15	6.0	6.0	2.4	6.0	2.5					
BR080	750	76	1.4	3.1	6.6	6.0	2.5					
105	1700	170	0.6	7.5	8.2	0.6	2.0					
106	1700	150	1.0	4.0	8.7	0.9	0.3					
107	450	44	1.5	0.9	1.1	1.9	0.8					
108	710	76	2.7	2.5	6.8	0.4	0.2					
CELL BLDG	380	56	5.0	5.2	1.8	0.4	2.2					
PROCESS SOUTH	370	110	13.0	6.8	5.0	1.4	1.5					
	OCDF (ng/kg)	1234678HpCDF (ng/kg)	1234789HpCDF (ng/kg)	123478HxCDF (ng/kg)	123678HxCDF (ng/kg)	123789HxCDF (ng/kg)	234678HxCDF (ng/kg)	23478PeCDF (ng/kg)	23478PeCDF (ng/kg)	2378TCDF (ng/kg)	PCDD/F TEQ (ng/kg)	Aroclor 1268 (mg/kg)
TEF	0.0003	0.01	0.01	0.1	0.1	0.1	0.1	0.03	0.3	0.1		
1718	1560	1210	187	700	192	15.9	120	293	106	250	214	56.0
36	2870	2000	372	1370	413	33.0	185	676	209	359	393	55.0
61	22200	21000	3800	11900	2770	270	600	5050	1670	2300	2768	1300
68	3960	4860	608	2640	734	387	384	1240	401	682	762	330
100	200	140	24.0	110	17	3.7	9.3	24.0	6.8	6.5	22.5	1.1
101	38.5	29.7	1.5	11.8	2.0	3.0	3.0	0.69	0.69	0.86	6.6	0.09
102	28.6	36.5	6.9	12.1	1.1	2.0	3.9	0.41	0.42	2.8	7.4	0.13
110	11.0	21.0	0.29	8.0	0.2	0.36	0.31	0.35	0.36	0.4	2.8	0.25
111	1062.3	1101.1	97	479	139	5.5	141.4	170	53.2	154	138	6.1
117	34.9	26.1	2.713	12.1	0.99	1.5	1.5	0.75	0.8	0.85	6.9	11
118	46.4	38.7	2.551	8.7	2.153	3.3	3.2	0.84	0.8435	1.8	9.4	10.00
BR048	58.0	37.0	3.4	10	4.6	6.0	7.4	6.2	4.60	10	20.4	1.4
C-15	128	145	9.9	68.0	17.8	0.1	27.5	31.9	18.7	32.3	53.6	0.1
C-6	2570	1520	799	5860	1650	328	731	6660	1020	4120	1878	7.6
C-8	260	277	35.10	188	46.5	6.5	48.9	98.5	35.5	104	124	2.20
EPA-E3	39100	43500	6050	20800	5640	349	3020	7280.0	2590	3510	4905	3800.00
EPA-F2	21800	25700	3000	21900	2900	204	2070	5400	1840	1300	3966	1188.00
EPA-H1	75900	92200	15700	49300	15700	661	7790	26100	6100	9660	12111	4000.00
GRID MARSH	390	260	50.0	240	61.0	53.0	52.0	170	120	220	119	6.10
BR003	4.8	2.7	6.0	6.0	6.0	6.0	6.0	6.0	6.0	2.5	15.1	0.01
BR008	38.0	25.0	6.0	10.0	3.2	6.0	3.5	5.2	2.9	10	13.6	0.59
BR010	3.7	1.7	6.0	6.0	6.0	6.0	6.0	6.0	6.0	2.5	15.1	0.05
BR022	12.5	6.0	6.0	6.0	6.0	6.0	6.0	6.0	6.0	2.5	15.2	0.05
BR028	12.5	2.0	6.0	6.0	6.0	6.0	6.0	6.0	6.0	2.5	15.1	0.25
BR030	13.0	12.0	6.0	6.0	6.0	6.0	6.0	1.8	6.0	2.5	15.4	0.11
BR032	60.0	43.0	3.0	10.0	3.9	6.0	6.7	5.1	4.0	10	19.7	0.61
BR041	16.0	15.0	6.0	4.4	2.4	6.0	3.0	6.0	1.3	2.5	11.2	0.12
BR052	12.5	1.6	6.0	6.0	6.0	6.0	6.0	6.0	6.0	2.5	14.7	0.10
BR055	12.5	2.2	2.2	6.0	6.0	6.0	6.0	6.0	6.0	2.5	15.1	0.25
BR074	12.5	6.0	6.0	6.0	6.0	6.0	6.0	6.0	6.0	2.5	14.9	0.04
BR080	7.8	5.9	6.0	2.0	6.0	6.0	6.0	6.0	6.0	2.5	14.9	0.05
105	20.0	34.0	0.3	9.7	1.7	0.6	0.5	0.5	0.6	3.9	8.6	0.99
106	18.0	21.0	0.7	5.7	0.7	1.1	1.0	0.4	0.4	1.9	5.9	0.16
107	0.9	0.6	0.8	0.7	0.4	0.7	0.6	1.3	1.3	0.55	4.3	0.58
108	3.0	3.5	0.6	1.3	0.2	0.3	0.3	0.2	0.3	0.135	3.1	0.60
CELL BLDG	4100	1700	340	1200	280	99.0	120	190	110	99.0	245	53.00
PROCESS SOUTH	5900	12000	340	3400	440	71.0	1300	130	340	53.0	764	450.00

Notes:

HpCDD Heptachlorodibenzo-p-dioxin  
 HxCDD Hexachlorodibenzo-p-dioxin  
 PeCDD Pentachlorodibenzo-p-dioxin  
 OCDD Octachlorodibenzo-p-dioxin

TCCD Tetrachlorodibenzo-p-dioxin  
 HpCDF Heptachlorodibenzofuran  
 HxCDF Hexachlorodibenzofuran  
 PeCDF Pentachlorodibenzofuran

OCDF Octachlorodibenzofuran  
 TCDF Tetrachlorodibenzofuran  
 TEQ Toxicity Equivalence  
 TEF Toxicity Equivalence Factor

TEF Source: Berg et al Berg, Martin Van Den, et al. "The 2005 World Health Organization Reevaluation of Human and Mammalian Toxic Equivalency Factors for Dioxins and Dioxin-Like Compounds." Toxicological Sciences, vol. 93, no. 2, 2006, pp. 223–241., doi:10.1093/toxsci/kfl055.

**Table 1b. Historical Sampling: Total PCDD/F Homologue Results**

Location	Total OCDF (ng/kg)	Total HpCDF (ng/kg)	Total HxCDF (ng/kg)	Total PeCDF (ng/kg)	Total TCDF (ng/kg)	Total OCDD (ng/kg)	Total HpCDD (ng/kg)	Total HxCDD (ng/kg)	Total PeCDD (ng/kg)	Total TCDD (ng/kg)	Total Furans (ng/kg)	Total Homologues (ng/kg)
<b>OU1 Locations</b>												
1718	1560	2330	2160	1380	1320	5770	3170	588	81.4	49.8	8750	18409
36	2870	3992	4099	2262	1245	6850	4880	713	75.1	51.8	14468	27038
61	22200	40700	31200	17300	11000	13100	5110	968	167	161	122400	141906
68	3960	13160	11600	6890	5240	14800	7210	1040	182	110	40850	64192
100	11	24.0	24.0	6.5	5	690	75.0	17.0	0.00	3.2	71	856
101	38.5	29.7	47.6	26.3	19.0	1387	498	1.4	9.3	0.77	161	2058
102	28.6	43.4	44.8	24.3	6.2	1795	649	70.2	8.8	7.5	147	2678
110	200	160	180	66.0	24	1700	670	43.0	0.00	5.6	630	3049
111	1062	1198	947	883	947	3286	1062	7.4	3.6	1.4	5036	9396
117	34.9	26.1	52.3	20.1	14.3	1481	495	1.649	7.2	0.78	148	2133
118	46.4	38.7	37.5	36.1	1.8	1803	730	40.6	2.3	1.5	161	2738
BR048	58.0	53.0	110.0	85.0	85.0	1500	740	310	18.0	22.0	391	2981
C-15	128	296	371	270	283	5860	2420	963	163	80.0	1348	10834
C-6	2570	3300	12080	15210	11550	8810	4410	987	149	123	44710	59189
C-8	260	541	765	550	710	5280	902	1360	187	99.4	2826	10654
EPA-E3	39100	72200	54400	30200	23300	14000	5890	990	154	94.2	219200	240328
EPA-F2	16000	17000	28000	11000	5700	16000	0.00	380	0	7.7	77700	94088
EPA-H1	75900	155000	137000	84500	55200	22000	7190	1270	58.4	85.8	507600	538204
GRID MARSH	390	540	800	860	1100	1600	470	190	15.0	15.0	3690	5980
<b>Regional Locations</b>												
BR003	4.8	3.2	3.3	6.0	2.5	65.0	25.0	15.0	6.0	2.4		
BR008	38.0	32.0	44.0	32.0	27.0	1500	720	230	11.0	15.0		
BR010	3.7	2.0	6.0	6.0	2.5	30.0	10.0	7.0	6.0	2.5		
BR022	12.5	6.0	6.0	6.0	2.5	130	25.0	23.0	2.1	2.9		
BR028	12.5	2.4	6.0	6.0	2.5	40.0	20.0	9.0	6.0	2.5		
BR030	13.0	31.0	21.0	14.0	11.0	2600	910	560	60.0	38.0		
BR032	60.0	59.0	88.0	71.0	69.0	2700	1100	600	43.0	43.0		
BR041	16.0	20.0	36.0	17.0	16.0	1700	720	440	51.0	30.0		
BR052	12.5	4.4	6.0	6.0	2.5	380	190	75.0	6.8	3.5		
BR055	12.5	2.6	2.6	6.0	2.5	80.0	30.0	25.0	1.5	1.3		
BR074	12.5	6.0	6.0	6.0	2.5	130	100	62.0	6.1	3.2		
BR080	7.8	7.0	6.1	5.4	2.4	750	290	180	13.0	8.1		
105	20.0	39.0	47.0	12.0	27.0	1700	200	58.0	9.3	14.0		
107	0.00	0.00	0.00	0.00	0.00	450	170	150	9.9	9.8		
108	3.0	3.50	6.8	0.00	0.00	710	76.0	49.0	17.0	13.0		
<b>Upland Locations</b>												
CELL BLDG	4100	2800	2500	720	380	120	42.0	4.5	18.0	380		
PROCESS SOUTH	5900	16000	13000	2900	940	370	410	190	19.0	16.0		
ES	82	21.07	16.7	5.96	2.32	8.35	3.23	0.26	0.04*	0.1*		

Notes:

Total homologues are reported from the laboratory report

\* 1/2 detection limit

OCDF Octachlorodibenzofuran

HpCDF Heptachlorodibenzofuran

HxCDF Hexachlorodibenzofuran

PeCDF Pentachlorodibenzofuran

TCDF Tetrachlorodibenzofuran

OCDD Octachlorodibenzo-p-dioxin

HpCDD Heptachlorodibenzo-p-dioxin

HxCDD Hexachlorodibenzo-p-dioxin

PeCDD Pentachlorodibenzo-p-dioxin

TCDD Tetrachlorodibenzo-p-dioxin

Table 2a. 2018 Co-location Sampling: PCDD/F Congeners and Aroclor 1268 Results

	OCDD (ng/kg)	1234678HpCDD (ng/kg)	1234789HxCDD (ng/kg)	123678HxCDD (ng/kg)	123789HxCDD (ng/kg)	12378PeCDD (ng/kg)	2378TCDD (ng/kg)					
TEF	0.0003	0.01	0.1	0.1	0.1	1	1					
D1-1A	4420	438	9.5	17.3	25.0	5.5	3.3					
D1-1B	4540	490	9.0	18.2	24.9	5.0	3.4					
D1-2A	4020	407	9.0	14.8	24.7	4.8	2.8					
D1-2B	3590	371	8.5	14.5	22.6	4.6	3.1					
D2-1A	4200	448	9.1	18	25.40	5.36	6.79					
D2-1B	3540	423	10.1	18.5	24.7	5.89	5.91					
EC-1A	4820	450	8.96	15.8	26.6	4.76	4.14					
EC-1B	4010	397	7.36	14.3	21.1	3.92	4.67					
EC-2A	5110	484	9.02	19.6	26.6	5.25	10.80					
EC-2B	2360	183.0	4.3	7.09	15.1	2.41	1.02					
EC-3A	3700	349.0	6.8	14.0	22.1	3.87	9.46					
EC-3B	6950	653.0	9.75	20.6	29.1	5.52	37.20					
EC-4A	6050	595	10.3	20.5	29.7	5.6	41.10					
EC-4B	4240	429	8.0	16.5	24.1	4.1	4.7					
LC-1A	4550	443.0	5.41	14.7	11.4	2.74	1.8					
LC-1B	8520	815	12.1	26.6	21.1	5.18	8.1					
MC-1A	5540	512	9.45	17.6	26.1	4.7	5.8					
MC-1B	5610	537.0	10.4	20.5	30.2	5.55	5.8					
MC-2A	4670.0	446.0	8.1	15.5	23.5	4.2	4.3					
MC-2B	4560	459	8.3	16.0	23.6	4.6	7.1					
MC-3A	2440.0	245.0	4.1	8.5	11.5	2.1	3.1					
MC-3B	2790	284.0	5.0	9.8	14.1	2.7	3.4					
PC-1A	20000	1960.0	19.1	60.0	46.4	8.5	23.6					
PC-1B	9760	949	11.1	31.5	30.6	5.7	14.0					
PC-2A	1890	154	1.8	4.6	7.3	1.0	1.3					
PC-2B	2150	218	1.3	7.1	11.6	0.8	0.8					
PC-3A	909	87.9	1.6	3.4	4.3	0.9	1.5					
PC-3B	615	57.2	1.2	2.1	2.9	0.6	0.8					
<b>EPA Split Samples</b>												
D1-1A	2900	320	9.3	16	21	5.6	3.7					
D2-1A	4100	450	12	26	26	7.2	24					
EC-2B	1100	120	5.2	6.9	13	3.3	1.7					
EC-4A	2400	290	9.7	17	18	5.9	39					
EC-4B	5400	580	15	24	28	6.2	9.8					
LC-1A	4800	490	9	16	12	4.6	2.8					
LC-1B	7200	760	15	30	23	5.9	11					
MC-3A	2000	210	5	9.1	11	2.7	3.9					
MC-3B	2000	220	6.1	11	16	3.1	3.6					
PC-1A	6900	810	17	41	35	8.2	19					
PC-1B	4200	450	8.6	21	20	5.3	13					
PC-2B	1800	190.0	1.0	7.3	12.0	0.85	0.9					
<b>EPA Split Samples</b>												
	OCDF (ng/kg)	1234678HpCDF (ng/kg)	1234789HxCDF (ng/kg)	123678HxCDF (ng/kg)	123789HxCDF (ng/kg)	234678HxCDF (ng/kg)	12378PeCDF (ng/kg)	23478PeCDF (ng/kg)	2378TCDF (ng/kg)	PCDD/F TEQ (ng/kg)	Aroclor 1268 (mg/kg)	
TEF	0.0001	0.01	0.01	0.1	0.1	0.1	0.03	0.3	0.1			
D1-1A	125	114	12.9	75.1	20.4	1.7	16.7	40.2	16.4	35.3	41.9	2.3
D1-1B	166	168	20.3	110	28.8	2.5	21.5	61.4	21.4	52	51.5	5.1
D1-2A	53.5	56.3	4.18	26.6	7.75	0.698	9.14	13.5	6.87	16.7	26.9	1.37
D1-2B	51.4	62.1	5.06	31.4	8.73	0.708	9.97	15.3	7.85	19.7	27.6	2.29
D2-1A	190	256	28.8	305	97.5	6.48	52.3	215.0	90.0	131	118.7	3.03
D2-1B	124.0	196.0	13.9	145.0	41.2	2.94	47.6	81.00	45.00	68.8	71.0	3.22
EC-1A	90.2	107.0	8.9	63.8	17.9	1.4	16.5	33.80	13.70	36.2	39.9	4.49
EC-1B	90.7	102.0	9.32	65.6	18.8	1.38	14.4	38.30	14.20	46.6	39.2	4.58
EC-2A	162.0	198.0	20.2	159	44.9	3.6	28.6	97.20	33.10	142	80.8	12.6
EC-2B	21	24.2	2.72	18.3	4.9	0.35	3.46	10.5	3.7	11.1	14.1	5.67
EC-3A	344.0	407.0	47.5	402.0	110	9.30	54.8	244.00	77.7	199.00	134.9	24.40
EC-3B	937.0	869.0	248	2640	779	68.40	139	2310	702.00	1520	863.1	22.1
EC-4A	985.0	881.0	251.0	2340.0	691	67.9	133.0	1800.00	574.0	1140.00	735.4	28.8
EC-4B	305.0	440.0	45.6	377.0	101.0	6.57	68.6	219	72.90	160.0	123.9	7.7
LC-1A	145.0	89.5	6.23	27.2	8.15	0.638	9.26	13.0	6.9	18.3	23.3	0.72
LC-1B	227.0	310.0	30.1	276.0	78.6	5.76	43.5	154.0	58.5	164	112.3	0.96
MC-1A	221.0	248.0	26.70	165.0	43.5	3.39	31.8	81.5	29.4	69.8	68.0	9.35
MC-1B	137.0	151.0	15.9	86.0	21.8	1.65	21.3	42.0	17	47.3	50.4	2.86
MC-2A	159.0	175.0	19.1	125.0	33.2	2.6	24.2	61.6	22.1	52.1	53.2	4.98
MC-2B	220.0	242.0	26.9	164.0	42.2	3.2	32.2	86.7	29.6	84	69.2	14.2
MC-3A	131.0	149.0	15.0	105.0	29.4	2.2	19.9	54.2	19.7	57.3	41.3	5.68
MC-3B	196.0	248.0	25.4	160.0	41.0	3.3	31.2	76.0	27.7	63.9	56.0	18.00
PC-1A	1470.0	1890.0	185.0	1190.0	281.0	25.0	263.0	549.0	225.0	297	380.7	31.1
PC-1B	448.0	517.0	46.2	285.0	72.9	5.7	71.1	130.0	54.3	124	121.2	24.5
PC-2A	106.0	118.0	10.6	58.5	12.2	1.1	10.6	24.0	8.4	12.4	19.8	1.24
PC-2B	22.0	25.0	2.7	17.7	4.7	0.4	3.2	10.0	3.4	8.89	11.6	1.03
PC-3A	33.2	36.6	4.5	22.8	5.8	0.5	5.0	11.7	4.3	11.5	11.0	1.89
PC-3B	23.4	24.4	2.7	13.4	3.5	0.3	3.1	7.2	2.7	7.29	6.9	0.60
<b>EPA Split Samples</b>												
D1-1A	110	91	13	67	22	16	23	46	42	55	51.3	2.29
D2-1A	400	460	92	1000	340	210	170	1000	850	570	560.0	3.03
EC-2B	10	13	1.6	14	4.3	2.8	4.2	12	11	15	16.9	5.67
EC-4A	540	490	140	1500	470	370	210	1700	1500	980	913.3	28.80
EC-4B	520	690	73	680	200	110	160	410	350	300	300	7.66
LC-1A	140	94	6.7	33	11	5.3	15	15	16	19	32.0	0.72
LC-1B	240	360	27	310	94	50	76	180	150	180	158.8	0.96
MC-3A	140	150	17	110	36	19	33	73	65	66	61.6	5.68
MC-3B	180	190	22	130	40	23	39	76	66	61	66.3	18.00
PC-1A	530	580	75	430	130	86	150	270	250	190	240.0	31.10
PC-1B	230	240	26	160	50	29	65	100	95	110	104.6	24.50
PC-2B	21	22	2.6	17.0	5.0	2.7	6.3	11.0	9.5	8.4	13.5	1.03

Notes:

HxCDD Heptachlorodibenzo-p-dioxin	TCDD Tetrachlorodibenzo-p-dioxin	OCDF Octachlorodibenzofuran
HxCDD Hexachlorodibenzo-p-dioxin	HxCDF Heptachlorodibenzofuran	TCDF Tetrachlorodibenzofuran
PeCDF Pentachlorodibenzo-p-dioxin	HxCDF Hexachlorodibenzofuran	TEQ Toxicity Equivalence
OCDD Octachlorodibenzo-p-dioxin	PeCDF Pentachlorodibenzofuran	TEF Toxicity Equivalence Factor

TEF Source: Berg et al Berg, Martin Van Den, et al. "The 2005 World Health Organization Reevaluation of Human and Mammalian Toxic Equivalency Factors for Dioxins and Dioxin-Like Compounds." Toxicological Sciences, vol. 93, no. 2, 2006, pp. 223–241., doi:10.1093/toxsci/kf055.

**Table 2b. 2018 Co-location Sampling: Total Homologue Results**

Location	Total OCDF (ng/kg)	Total HpCDF (ng/kg)	Total HxCDF (ng/kg)	Total PeCDF (ng/kg)	Total TCDF (ng/kg)	Total OCDD (ng/kg)	Total HpCDD (ng/kg)	Total HxCDD (ng/kg)	Total PeCDD (ng/kg)	Total TCDD (ng/kg)	Total Furans (ng/kg)	Total Homologues (ng/kg)
D1-1A	125	243	315	284	239	4420	1620	703	101	64.0	1206	8114
D1-1B	166	341	421	367	346	4540	1830	771	100	61.6	1641	8944
D1-2A	53.5	120	156	127	108	4020	1560	658	91.2	51.2	565	6945
D1-2B	51.4	125	165	135	124	3590	1370	592	84.9	48.1	600	6285
D2-1A	190	448	1040	1210	943	4200	1640	643	101	55.6	3831	10471
D2-1B	124	328	764	956	990	3540	1380	571	83.7	45.4	3162	8782
EC-1A	90.2	198	277	235	199	4820	1640	719	102	57.1	999	8337
EC-1B	90.7	188	264	235	224	4010	1530	630	93.5	54.7	1002	7320
EC-2A	162	335	527	514	492	5110	1730	757	107	69.0	2030	9803
EC-2B	21.0	39.2	59.0	55.3	55.4	2360	644	426	65.6	34.7	230	3760
EC-3A	344	644	1080	992	750	3700	1180	515	88.9	49.8	3810	9344
EC-3B	937	1600	5420	7470	5310	6950	2600	735	124	82.4	20737	31228
EC-4A	985	1600	4870	5860	3750	6050	2190	744	128	80.2	17065	26257
EC-4B	305	696	1200	738	507	4240	1410	636	56.0	10.3	3446	9798
LC-1A	145	240	176	107	60.2	4550	1270	240	38.9	11.6	728	6839
LC-1B	227	628	876	679	548	8520	3160	636	75.4	44.4	2958	15394
MC-1A	221	435	578	457	398	5540	1780	720	122	57.4	2089	10308
MC-1B	137	287	383	305	297	5610	1950	880	124	67.3	1409	10040
MC-2A	159	312	426	326	292	4670	1600	663	91.5	54.8	1515	8594
MC-2B	220	423	567	456	423	4560	1650	673	87.9	55.9	2089	9116
MC-3A	131	250	355	308	314	2440	855	313	41.1	25.8	1358	5033
MC-3B	196	397	514	393	372	2790	916	355	56.9	28.4	1872	6018
PC-1A	1470	3670	4110	2510	1550	20000	5890	1330	145	91.3	13310	40766
PC-1B	448	1050	1250	999	864	9760	2880	899	134	76.8	4611	18361
PC-2A	106	191	168	106	78.3	1890	562	263	68.1	102	649	3534
PC-2B	22.0	42.0	56.0	42.9	43.8	2150	606	342	95.4	73.2	207	3473
PC-3A	33.2	69.5	87.1	63.8	62.6	909	307	130	16.6	12.2	316	1691
PC-3B	23.4	44.0	53.4	42.7	42.7	615	202	85.7	10.7	8.0	206	1128
<b>EPA Split Samples</b>												
D1-1A	110	210	320	330	290	2900	1100	620	140	64		
D2-1A	400	830	2600	3500	2300	4100	1600	720	140	84		
EC-2B	10	23	51	66	86	1100	420	370	91	50		
EC-4A	540	950	3500	5700	4200	2400	1600	600	150	110		
EC-4B	520	1200	2200	2400	2200	5400	2100	830	150	71		
LC-1A	140	250	220	140	120	4800	1300	280	56	31		
LC-1B	240	670	1000	820	720	7200	2300	610	110	53		
MC-3A	140	260	410	400	400	2000	630	310	63	33		
MC-3B	180	320	460	410	380	2000	670	350	69	36		
PC-1A	530	1300	1900	1600	1300	6900	2600	910	170	98		
PC-1B	230	530	790	750	790	4200	1400	590	120	80		
PC-2B	21	38	59	54	45	1800	500	320	88	70		

Notes:

Total homologues are reported from the laboratory report

OCDF Octachlorodibenzofuran

HpCDF Heptachlorodibenzofuran

HxCDF Hexachlorodibenzofuran

PeCDF Pentachlorodibenzofuran

TCDF Tetrachlorodibenzofuran

OCDD Octachlorodibenzo-p-dioxin

HpCDD Heptachlorodibenzo-p-dioxin

HxCDD Hexachlorodibenzo-p-dioxin

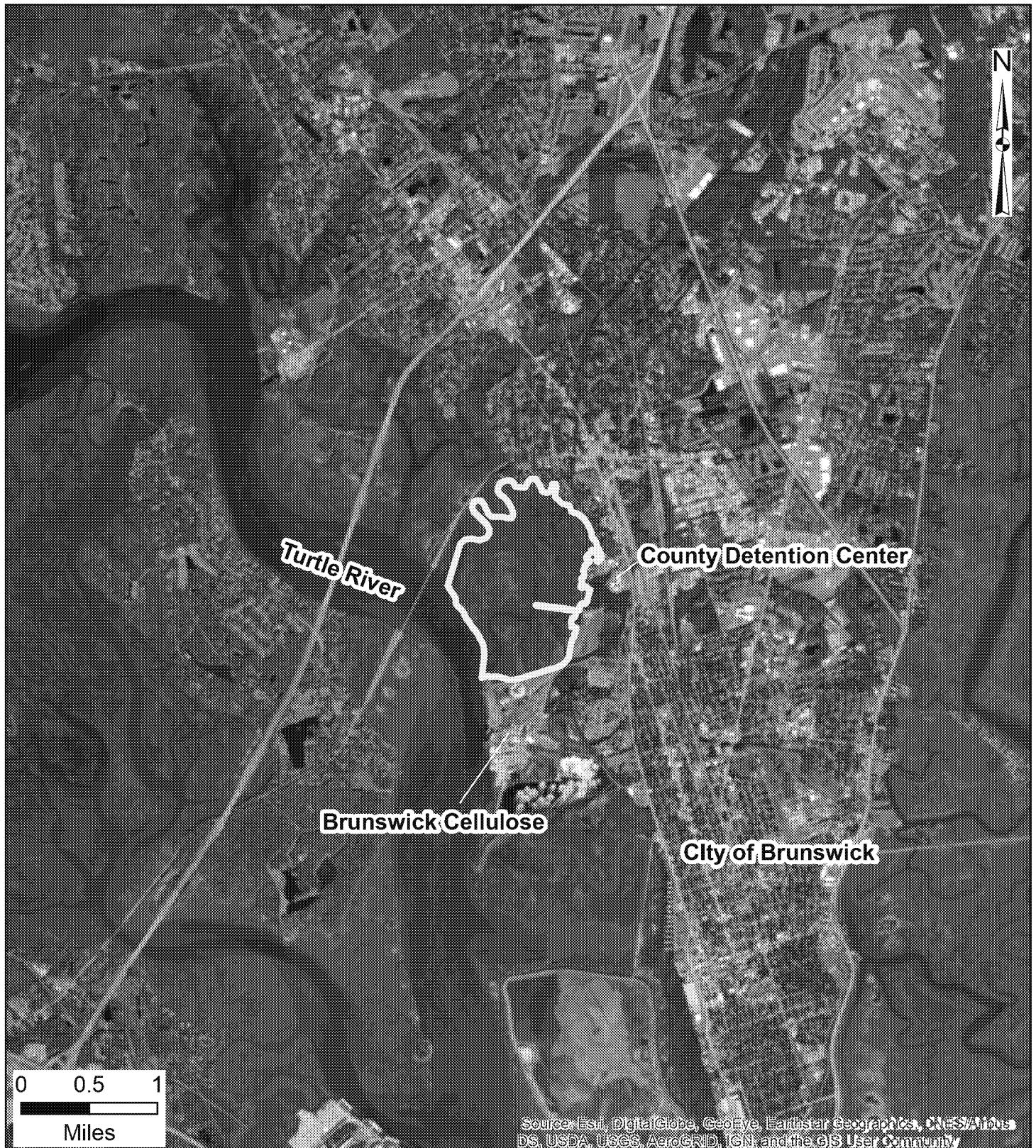
PeCDD Pentachlorodibenzo-p-dioxin

TCDD Tetrachlorodibenzo-p-dioxin

\* Total homologues are reported from the laboratory report

EPS

## FIGURES

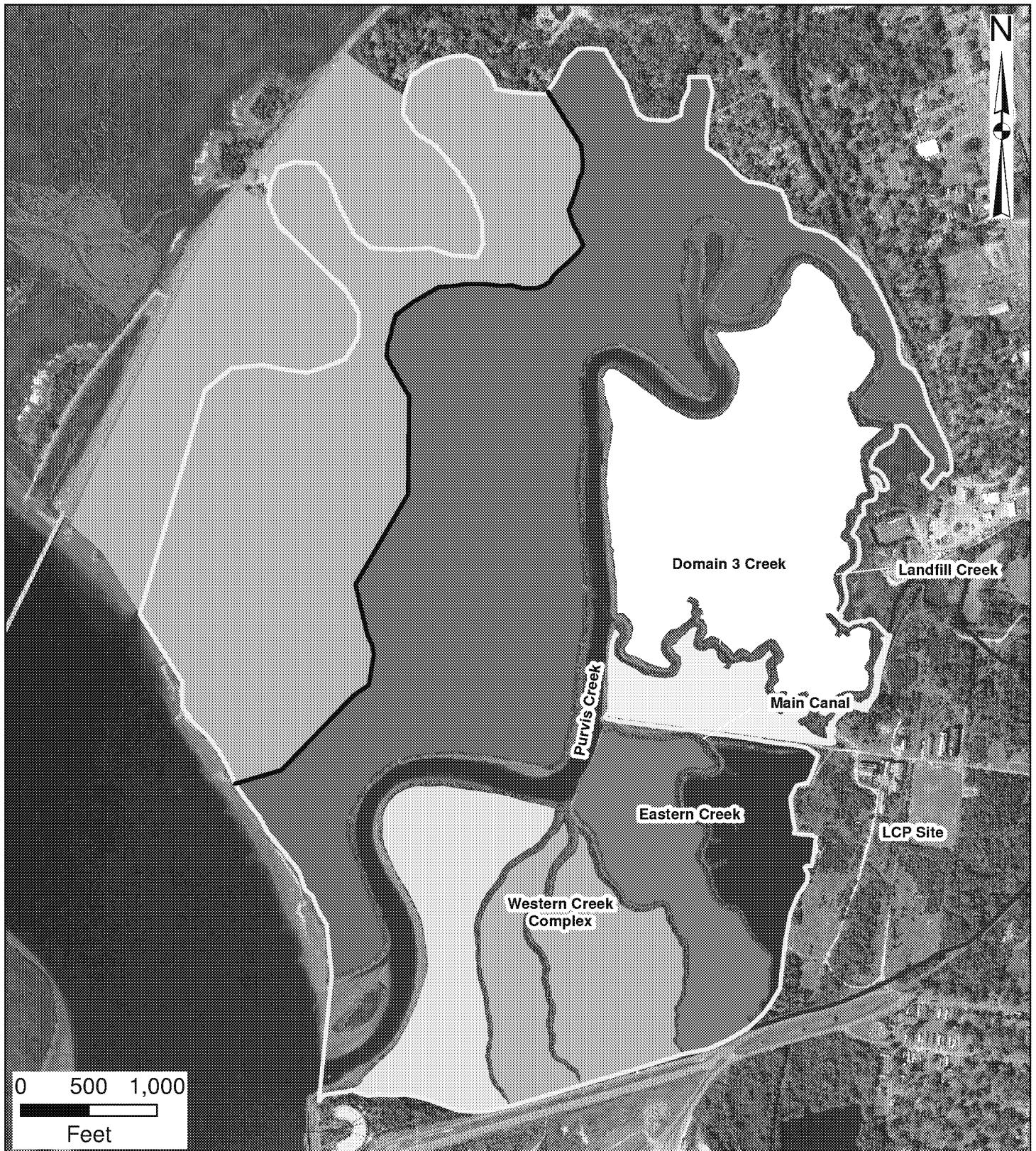


OU1 (LCP Marsh)

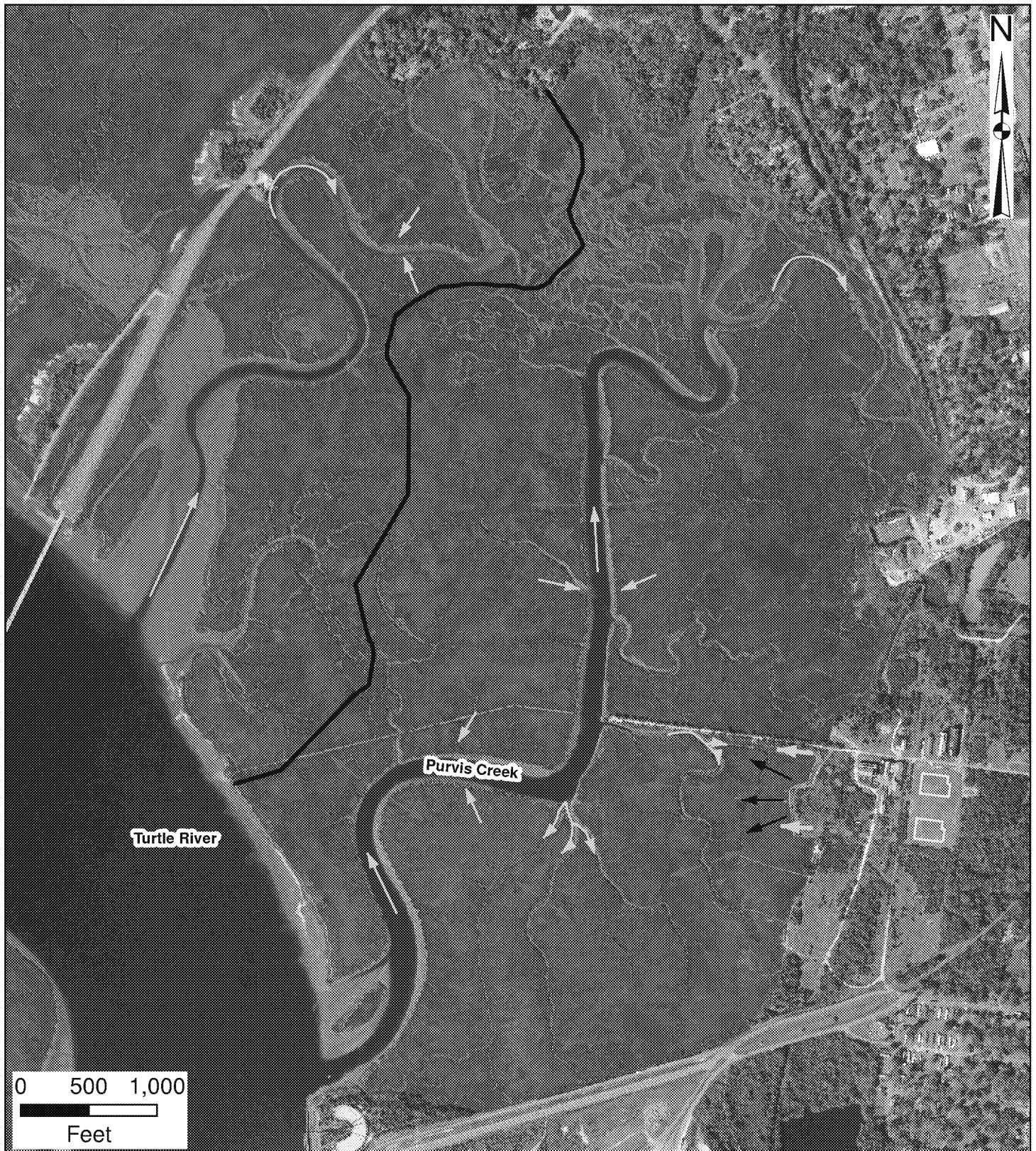
LCP Uplands

### Site Location Map

*LCP Chemicals Site  
Brunswick, GA*



Primary Tidal Node	Domain Name	OU1 Features
OU1 (LCP Marsh)	Domain 1	OU1 Chemicals Site
LCP Uplands	Domain 2a	Brickfield Hill
	Domain 2b	Brickfield Hill
	Domain 2c	Brickfield Hill
	Domain 2d	Brickfield Hill
	Domain 3a	Brickfield Hill
	Domain 3b	Brickfield Hill
	Domain 4a	Brickfield Hill
	Domain 4b	Brickfield Hill



- ◆— Primary Wastewater Discharge Point
- \* — Process Piping
- ..... Cell Buildings
- Primary Tidal Node
- ..... Ebb tide- early stage
- Ebb tide- late stage
- Surface erosion and tidal mixing
- ..... Flood tide- early stage
- Flood tide- late stage

## OU1 Conceptual Site Model Features

*LCP Chemicals Site  
Brunswick, GA*



**Aroclor 1268**

●	○	10-50 mg/kg
●	●	<1 mg/kg
●	●	50-100 mg/kg
●	●	1-10 mg/kg
●	●	>100 mg/kg

**Aroclor 1268 Condition in OU1  
Prior to the 1998-99 Removal Action**

*LCP Chemicals Site  
Brunswick, GA*



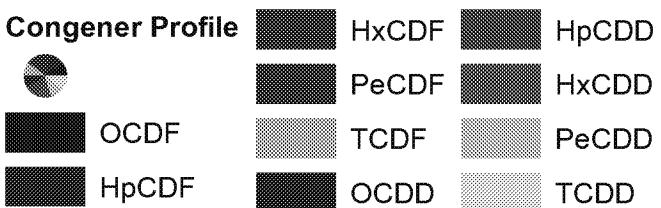
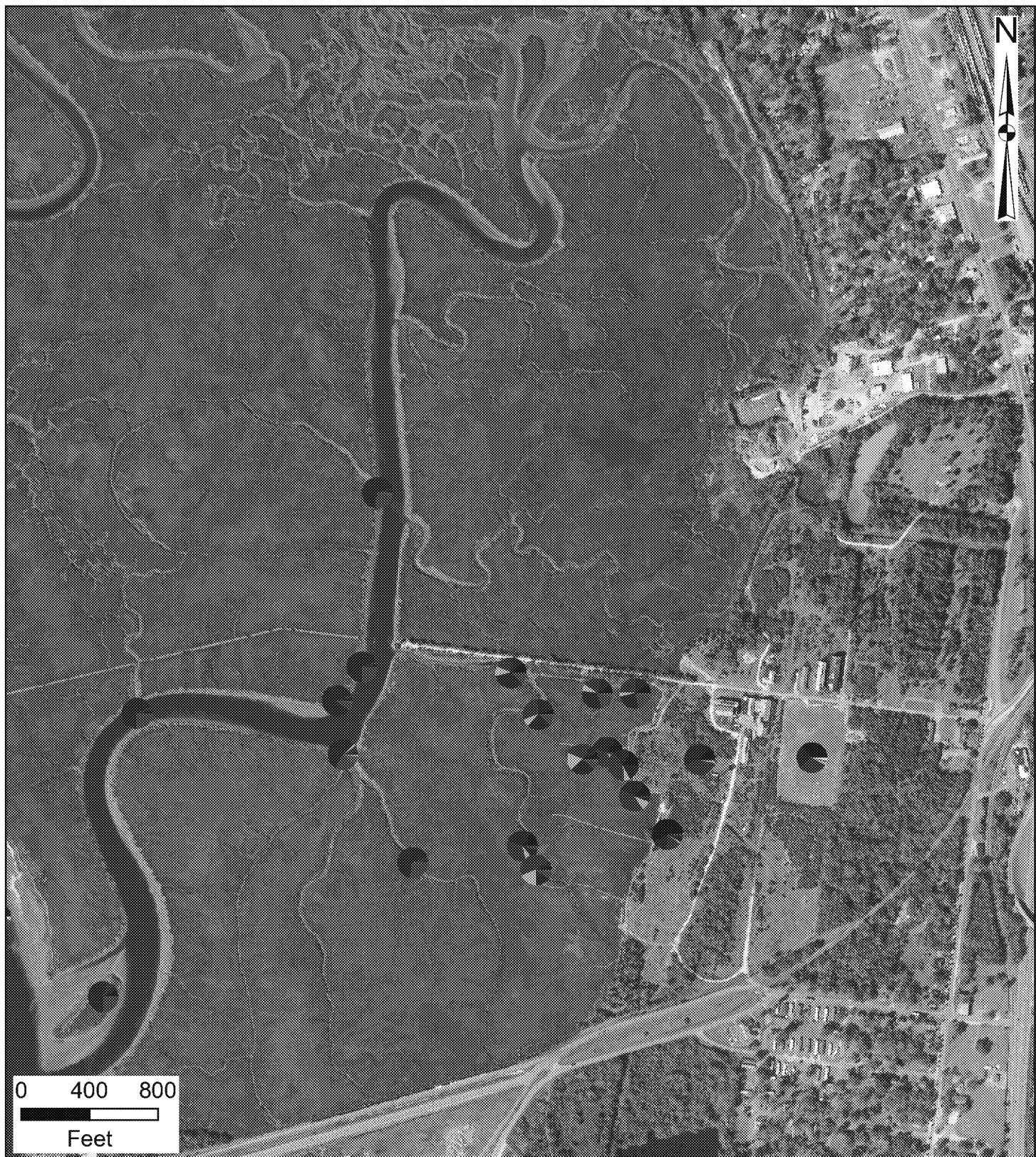
Environmental Planning Specialists, Inc.  
TEQ

- <10 ng/kg
- 10-100 ng/kg
- 100-260 ng/kg
- 260-1000 ng/kg
- >1000 ng/kg

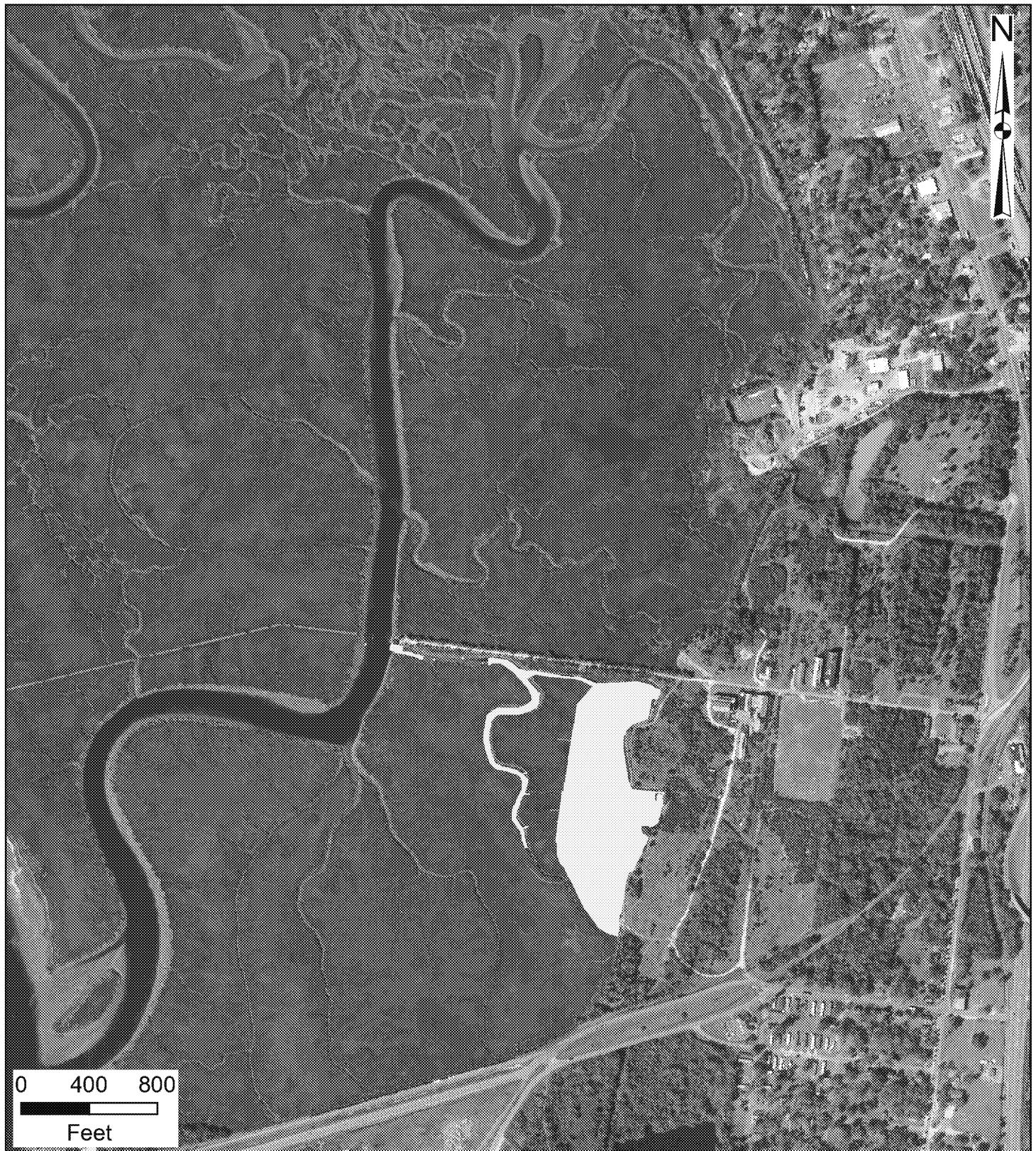
**Dioxin TEQ Condition in OU1 Prior  
to the 1998-99 Removal Action**

*LCP Chemicals Site  
Brunswick, GA*

**Figure No. 5**



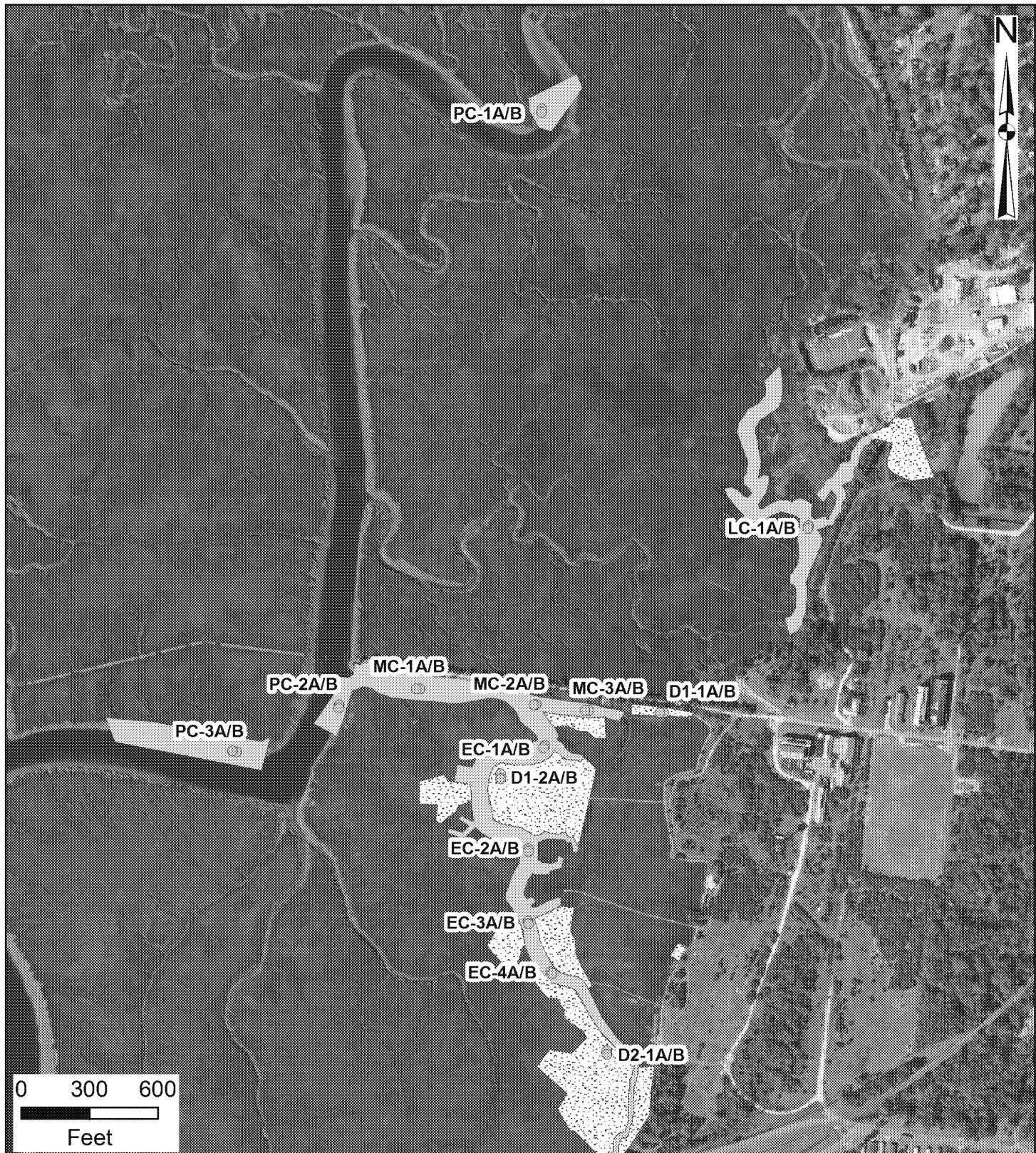
**PCDD/F Congener Profile of Soil/Sediment Locations in OU1 Prior to the 1998-99 Removal Action**  
*LCP Chemicals Site  
Brunswick, GA*



Marsh Removal Area

### Marsh Removal Action Areas (1998/1999)

*LCP Chemicals Site  
Brunswick, GA*



● Sediment Sampling Location

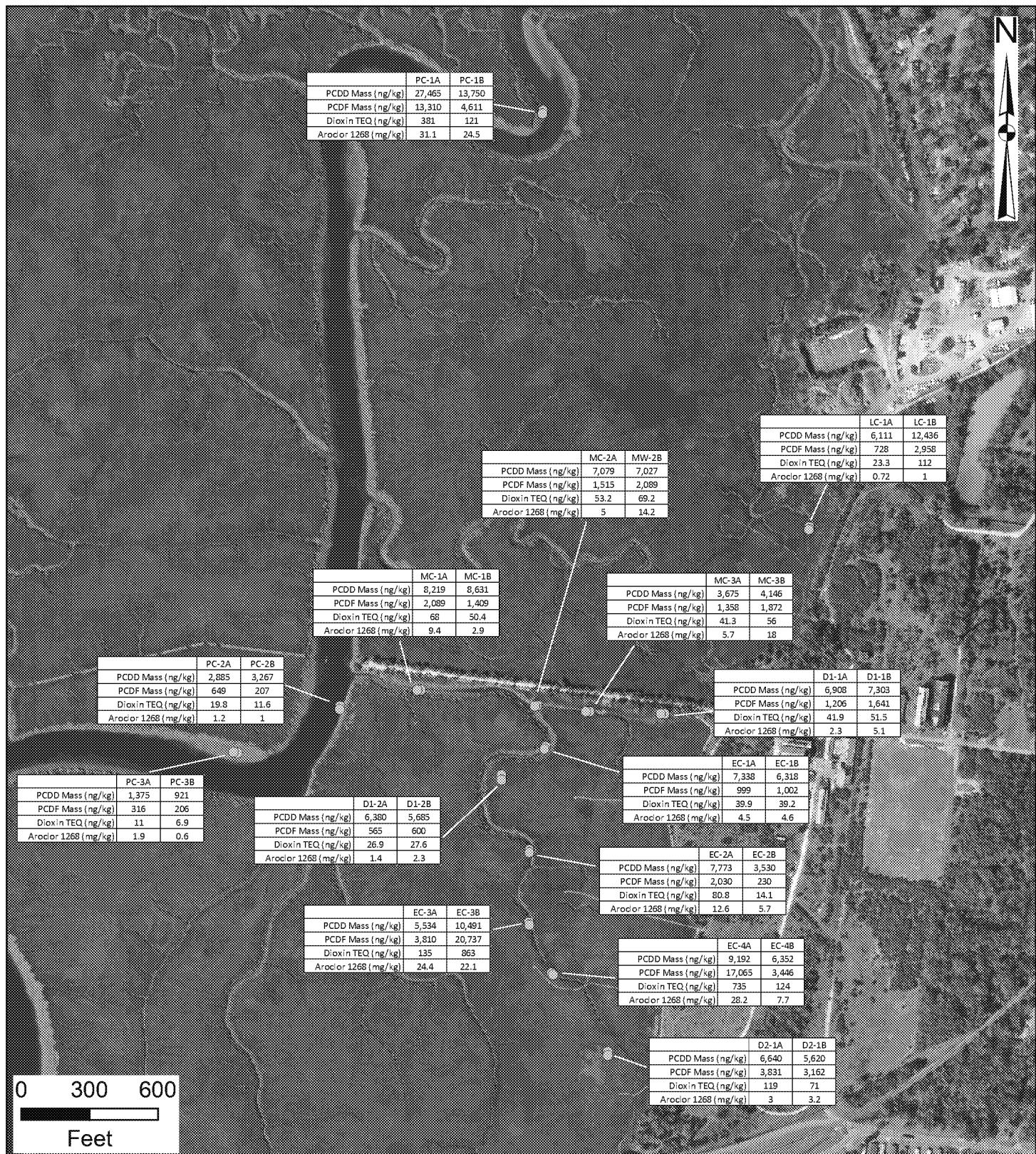
For each paired sample set, sample A is the northern or eastern sample location, sample B is the southern or western sample location.

#### OU1 Selected Remedy

- [Solid Gray Box] Cap
- [Dotted Gray Box] Dredge
- [Cross-hatched Box] Thin Cover

**Co-location Study Sampling Locations**

*LCP Chemicals Site  
Brunswick, GA*

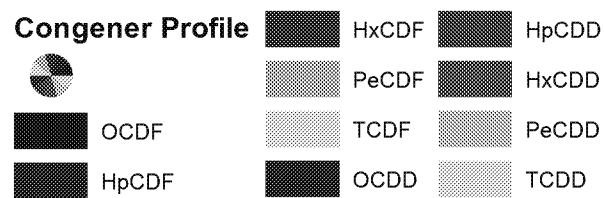
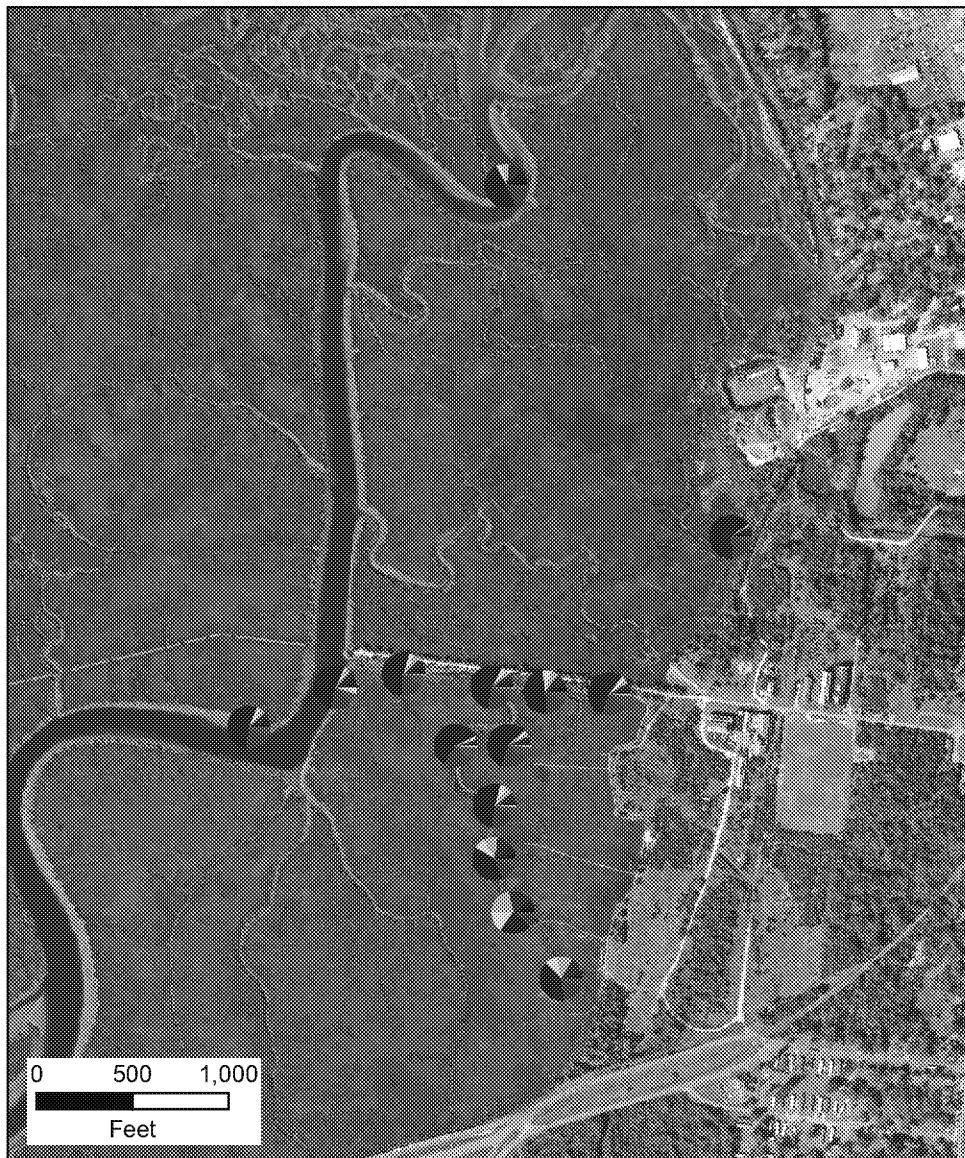


● Sediment Sampling Location

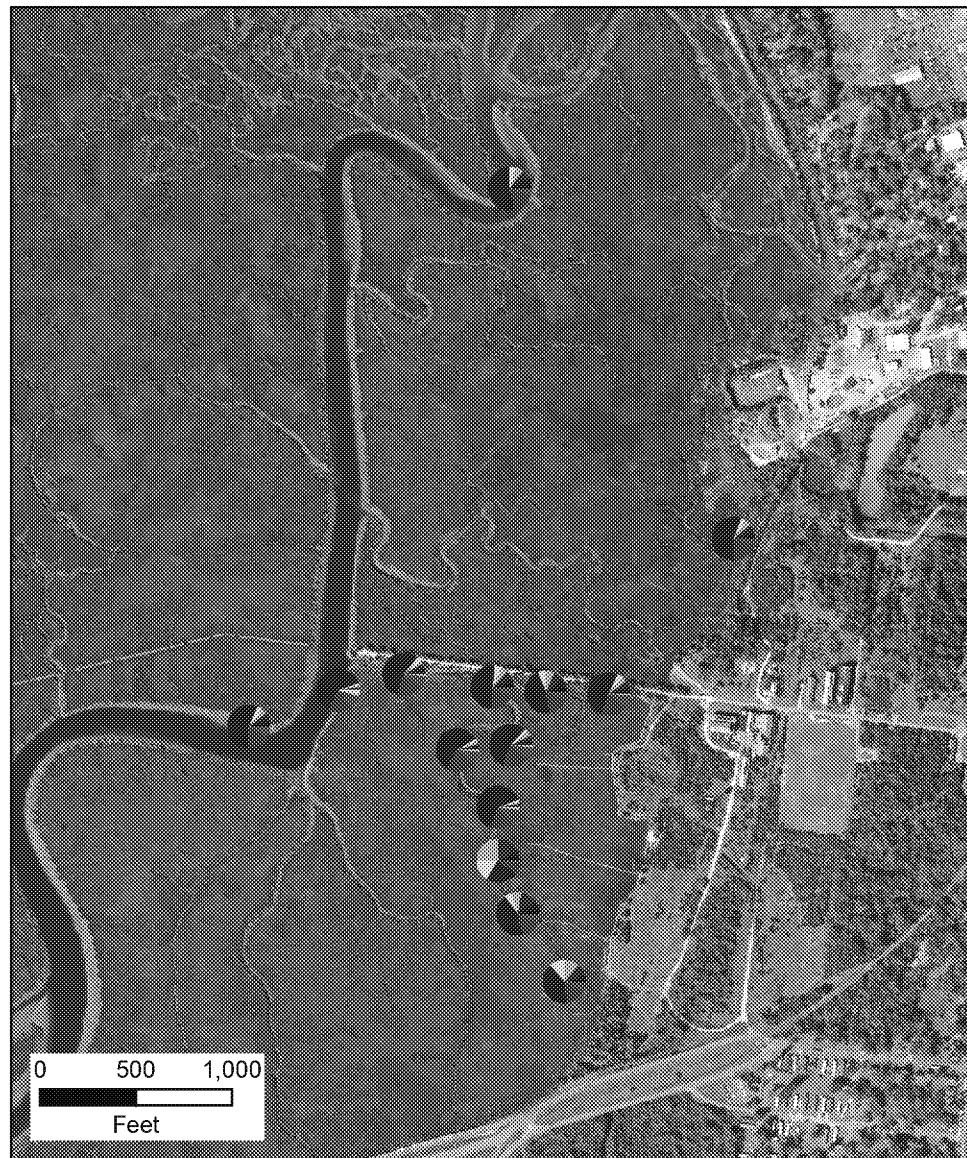
### Co-location Study Sampling Results

*LCP Chemicals Site  
Brunswick, GA*

**Location A**



**Location B**



**PCDD/F Congener Profiles for  
Co-location Study Sampling  
LCP Chemicals Site  
Brunswick, GA**

**Location A**



**PCDD/F Congener Profile**



Dioxin Portion of Total PCDD/F

- Notes:
1. The figure depicts both the total PCDD/F mass and Aroclor 1268 mass (concentration).
  2. Total PCDD/F relative mass concentration is depicted by the proportional size of the circle.
  3. Aroclor 1268 concentration is depicted by the value posted at each sampling location.
  4. Aroclor 1268 results in mg/kg.

**Location B**



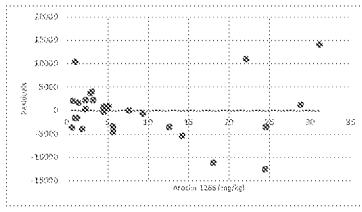
**2018 Co-location Study Results**  
**Total PCDD/F Mass Concentration**  
**and Corresponding Aroclor 1268**  
**Concentration**  
**LCP Chemicals Site**  
**Brunswick, GA**

**APPENDIX B**  
**Testing of Linear Regression**  
**Assumptions for**  
**Co-location Cases 1-3**

**Case 1a: Furan Congener Concentration and Aroclor 1268 (Co-location Study Data)**

Location	PCDD/F (ng/kg)	Aroclor 1268 (mg/kg)	Pred PCDD/F (ng/kg)	Pred PCDD/F <sup>2</sup> (ng/kg)	Residual PCDD/F	Residual <sup>2</sup>
D1-1A	3114.0	2.29	5911.96	349513111.31	2202.04	4848865.16
D1-1B	8943.5	5.12	7951.19	63221397.64	992.31	984682.23
D1-2A	6944.9	1.37	5249.04	27552369.75	1695.86	2875957.67
D1-2B	6285.4	2.29	5911.96	349513111.31	373.44	139454.89
D2-1A	10470.6	3.03	6445.19	41540452.57	4025.41	16203939.14
D2-1B	8782.1	3.22	6582.10	43324006.55	2200.00	4840011.32
EC-1A	9337.3	4.49	7497.23	56208407.96	840.07	705723.17
EC-1B	7319.9	4.58	7562.09	57185029.19	242.18	58562.36
EC-2A	9803.0	12.6	13341.08	177984511.38	-3538.08	12518035.50
EC-2B	3760.2	5.67	8347.50	6989827.40	-4587.30	21043360.39
EC-3A	9343.7	24.4	21843.86	4717154191.77	-12501.16	15625384.04
EC-3B	31228.4	22.1	20185.54	407496343.07	11041.86	121922701.85
EC-4A	26257.2	28.8	25014.39	625719502.90	1242.81	1544586.84
EC-4B	9798.3	7.66	9781.45	95676724.54	16.85	284.03
LC-1A	6838.7	0.721	4781.38	22861618.21	2057.32	4232955.47
LC-1B	15933.8	0.964	4956.48	24566713.75	10437.32	108937607.18
MC-1A	10309.4	9.35	10999.22	1209982783.04	-690.82	477228.66
MC-1B	10040.3	2.86	6322.69	39976417.81	3717.61	13820618.83
MC-2A	8594.3	4.98	7850.31	61627336.50	743.09	553524.02
MC-2B	9115.8	14.2	14494.00	210076103.82	-5378.20	28925060.40
MC-3A	5032.9	5.68	8354.71	69801179.25	-3321.81	11034421.70
MC-3B	6018.3	18	17232.18	296948178.06	-11213.88	12575120.60
PC-1A	40766.3	31.1	26671.71	711379934.02	14094.59	198657562.55
PC-1B	18360.8	24.5	21915.92	480307408.42	-3555.12	12638955.34
PC-2A	3534.4	1.24	5155.36	26577741.65	-1620.96	2627512.87
PC-2B	3473.3	1.03	5004.04	25040415.23	-1530.74	2343164.61
PC-3A	1691.0	1.89	5623.73	31626380.94	-3932.73	15466394.50
PC-3B	1127.6	0.604	4697.08	22062516.13	-3569.51	12741367.90

Test for Zero Conditional Mean of Errors



No discernable relationship between residuals and independent variable  
 $\text{Cov}(\hat{y}_i, x_i) = 0$

Tests for Homoscedasticity

BREUSCH-PAGAN SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.620776693
R Square	0.385363703
Adjusted R Square	0.361723845
Standard Error	43838769.96
Observations	28

$$\hat{y}^2 = q_0 + q_1 x_1$$

$H_0$  = homoscedasticity of residuals  
 $H_a$  = heteroscedasticity of residuals  
 $p < 0.05$   
**Status: Heteroscedastic**

ANOVA

	df	SS	MS	F	Significance F
Regression	1	3.13287E+16	3.13287E+16	16.30143927	0.000423921
Residual	26	4.95678E+16	1.932184E+15		
Total	27	8.12965E+16			

Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	-229567.4794	11420019.9	-0.20102196	0.984115326	2344619.61	-23703754.57	23244619.61
Aroclor 1268 (mg/kg)	3630705.783	899245.136	4.037504089	1782291	5479130.566	1782291	5479130.566

WHITE'S SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.643059799
R Square	0.413525905
Adjusted R Square	0.366607978
Standard Error	43670718.25
Observations	28

$$\hat{y}^2 = q_0 + \hat{Y} \times q_1 \hat{Y}^2 \times q_2$$

$H_0$  = homoscedasticity of residuals  
 $H_a$  = heteroscedasticity of residuals  
 $p < 0.05$   
**Status: Heteroscedastic**

ANOVA

	df	SS	MS	F	Significance F
Regression	2	3.36182E+16	1.68091E+16	8.813814385	0.001265974
Residual	25	4.76783E+16	1.90713E+15		
Total	27	8.12965E+16			

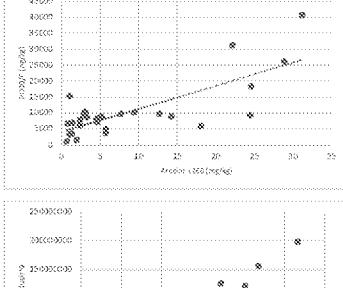
Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%	
Intercept	1787035.75	39306891.44	0.454649036	0.653285044	-63083201.98	98824873.47	-63083201.98	98824873.47
Pred PCDD/F (ng/kg)	-2588.756137	7071534772	-0.366081229	0.717384202	1175.34235	-17152.85463	11975.34235	-17152.85463
Pred PCDD/F <sup>2</sup>	0.26333361	1.09566779	0.231659605	0.758331804	0.231659605	0.758331804	0.231659605	0.758331804

Location	PCDD/F (ng/kg)	Aroclor 1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight	Weight X	Weight X <sup>2</sup>
D1-1A	3114.0	2.29	5911.96	2202.04	2382.2015	1.76215E-07	4.03533E-07	9.2409E-07	
D1-1B	8943.5	5.12	7951.19	992.31	3081.96997	1.05279E-07	5.3903E-07	2.75983E-06	
D1-2A	6944.9	1.37	5249.04	1695.86	2154.713139	2.15389E-07	2.95081E-07	4.04261E-07	
D1-2B	6285.4	2.29	5911.96	373.44	2382.20015	1.76215E-07	4.03533E-07	9.2409E-07	
D2-1A	10470.6	3.03	6445.19	4025.41	2565.179532	1.51972E-07	4.60476E-07	1.39524E-06	
D2-1B	8782.1	3.22	6582.10	2200.03	2612.159846	1.46555E-07	4.71907E-07	1.51954E-06	
EC-1A	9337.3	4.49	7497.23	840.07	2926.190829	1.16787E-07	5.24374E-07	2.35444E-06	
EC-1B	7319.9	4.58	7562.08	-242.18	2948.44492	1.15031E-07	5.26841E-07	2.41293E-06	
EC-2A	9803.0	12.6	13341.08	-3538.08	3538.08	4.913153824	4.11183E-08	5.18091E-07	6.52794E-06
EC-2B	3760.2	5.67	8347.50	-4587.304	4587.304	3217.36756747	9.65689E-08	5.47545E-07	3.10458E-06
EC-3A	9343.7	24.4	21843.86	-12501.59	12501.59	7849.306469	1.62307E-08	3.96023E-07	9.63311E-06
EC-3B	31228.4	22.1	20185.54	11041.86	11041.86	7290.589942	1.89654E-08	4.16926E-07	9.21407E-06
EC-4A	26257.2	28.8	25014.39	1242.314	1242.314	8937.287826	2.15195E-08	3.60563E-07	1.03842E-05
EC-4B	9798.3	7.66	9781.45	16.85	3710.031942	2.65151E-08	5.56511E-07	4.26287E-06	
LC-1A	6838.7	0.721	4781.38	2057.32	1994.235888	2.51447E-07	1.81293E-07	1.30713E-07	
LC-1B	15933.8	0.964	4956.48	10437.318	10437.318	2054.322132	2.36955E-07	2.28423E-07	2.202E-07
MC-1A	10309.4	9.35	10999.22	-690.817	690.817	4127.915691	5.86865E-08	5.48719E-07	5.13052E-06
MC-1B	10040.3	2.86	6322.69	3717.61	3717.61	2523.143189	1.57078E-07	4.49244E-07	1.28494E-06
MC-2A	8594.3	4.98	7850.31	743.92	743.92	3047.352388	1.07685E-07	5.36271E-07	2.67063E-06
MC-2B	9115.8	14.2	14494.00	-5378.202	5378.202	5327.167869	3.52377E-08	5.00375E-07	7.10532E-06
MC-3A	5032.9	5.68	8354.71	-3321.810	3321.810	3220.440332	9.64205E-08	5.47669E-07	3.11076E-06
MC-3B	6018.3	18	17232.18	-11213.884	11213.884	6266.789132	2.54633E-07	4.58334E-07	4.58202E-06
PC-1A	40766.3	31.1	26671.71	14094.593	14094.593	9506.003534	1.10663E-08	3.44163E-07	1.07035E-05
PC-1B	18360.8	24.5	21915.92	-3555.117	3555.117	7874.033318	1.61289E-08	3.05159E-07	9.68139E-06
PC-2A	3534.4	1.24	5155.36	-1620.96	1620.96	2122.256823	2.21961E-07	2.75232E-07	3.41287E-07
PC-2B	3473.3	1.03	5004.04	1530.74	1530.74	2070.61852	2.33233E-07	2.40233E-07	2.47437E-07
PC-3A	1691.0	1.89	5623.73	-3932.734	3932.734	2283.292754	1.91912E-07	3.62526E-07	6.85173E-07
PC-3B	1127.6	0.604	4697.08	-3569.505	3569.505	1965.305475	2.58905E-07	1.56378E-07	9.44526E-08

SUM 3.36348E-06 1.16445E-05 0.00010507

$$\text{OLS Error Variance } 15339$$

$$\text{Var} = \frac{\sum w_i}{(\sum w_i)(\sum w_i x_i^2) - (\sum w_i x_i)^2}$$



Case 1a: Furan Congener Concentration and Aroclor 1268 (Co-location Study Data)

Iteration #1	PredY <sub>i</sub>	Res <sub>i</sub>	WLS solution is asymptotic at Iteration #4.
DI-1A	8114.0	2.29	
DI-1B	8943.5	5.12	
DI-2A	8944.9	1.37	
DI-2B	6252.4	2.29	
DI-3A	10470.8	3.03	
DI-3B	8782.1	3.22	
EC-1A	8337.3	4.49	
EC-1B	7319.9	4.58	
EC-2A	9601.3	1.25	
EC-2B	3708.3	5.67	
EC-3A	9343.7	24.4	
EC-3B	31228.4	22.1	
EC-4A	20257.2	28.8	
EC-4B	7978.3	7.69	
LC-1A	6887.7	0.71	
LC-1B	15393.8	0.964	
MC-1A	10308.4	9.35	
MC-1B	10640.3	2.86	
MC-2A	8594.3	4.98	
MC-2B	9133.8	14.2	
MC-3A	5032.9	5.68	
MC-3B	6018.3	18	
PC-1A	40766.3	31.1	
PC-1B	18160.8	24.5	
PC-2A	3524.4	1.25	
PC-2B	3473.3	1.03	
PC-3A	16910.1	1.89	
PC-3B	1127.6	0.694	

Iteration #1	PredY <sub>i</sub>	Res <sub>i</sub>	WLS solution is asymptotic at Iteration #4.	Iteration #2	PredY <sub>i</sub>	Res <sub>i</sub>	WLS solution is asymptotic at Iteration #4.
DI-1A	8114.0	2.29		DI-1A	8114.0	2.29	
DI-1B	8943.5	5.12		DI-1B	8843.5	5.12	
DI-2A	8944.9	1.37		DI-2A	6944.9	1.37	
DI-2B	6252.4	2.29		DI-2B	6252.4	2.29	
DI-3A	10470.8	3.03		DI-3A	10470.8	3.03	
DI-3B	8782.1	5.22		DI-3B	8782.1	3.22	
EC-1A	8337.3	4.49		EC-1A	8337.3	4.49	
EC-1B	7319.9	4.58		EC-1B	7319.9	4.58	
EC-2A	9601.3	12.5		EC-2A	9800.0	12.6	
EC-2B	3708.3	5.67		EC-2B	3708.3	5.67	
EC-3A	9343.7	24.4		EC-3A	9343.7	24.4	
EC-3B	31228.4	22.1		EC-3B	31228.4	22.1	
EC-4A	20257.2	28.8		EC-4A	20257.2	28.8	
EC-4B	7978.3	7.69		EC-4B	7978.3	7.69	
LC-1A	6887.7	0.71		LC-1A	6887.7	0.71	
LC-1B	15393.8	0.964		LC-1B	15393.8	0.964	
MC-1A	10308.4	9.35		MC-1A	10308.4	9.35	
MC-1B	10640.3	2.86		MC-1B	10640.3	2.86	
MC-2A	8594.3	4.98		MC-2A	8594.3	4.98	
MC-2B	9133.8	14.2		MC-2B	9133.8	14.2	
MC-3A	5032.9	5.68		MC-3A	5032.9	5.68	
MC-3B	6018.3	18		MC-3B	6018.3	18	
PC-1A	40766.3	31.1		PC-1A	40766.3	31.1	
PC-1B	18160.8	24.5		PC-1B	18160.8	24.5	
PC-2A	3524.4	1.25		PC-2A	3524.4	1.25	
PC-2B	3473.3	1.03		PC-2B	3473.3	1.03	
PC-3A	16910.1	1.89		PC-3A	16910.1	1.89	
PC-3B	1127.6	0.694		PC-3B	1127.6	0.694	

Overall Fit	Multiple R	AIC	B-SIC	Observations
	0.529989367	20.33056889	20.81056889	28
R Square	0.279262896	AICc		
Adjusted R Square	0.253155571	B-SICc		
Standard Error	1.43692019			
Observations				

ANOVA	df	SS	MS	F	p-value	sig
Regression	1	20.93379891	20.93379891	10.16251603	0.003800262	yes
Residual	26	24.88952715				
Total	27	24.88952715				

coeff	std err	tstat	p-value	lower	upper	vif
Intercept	5354.574519	998.606187	5.36204679	1.2981105	3301.905945	7407.239492
X-Aro1268(mg/kg)	5667.7111097	178.291974	31.78485535	0.003800262	200.211916	933.209313

Iteration #2	PredY <sub>i</sub>	Res <sub>i</sub>	WLS solution is asymptotic at Iteration #4.	Iteration #3	PredY <sub>i</sub>	Res <sub>i</sub>	WLS solution is asymptotic at Iteration #4.
DI-1A	8114.0	2.29		DI-1A	8114.0	2.29	
DI-1B	8843.5	5.12		DI-1B	8843.5	5.12	
DI-2A	8944.9	1.37		DI-2A	6944.9	1.37	
DI-2B	6252.4	2.29		DI-2B	6252.4	2.29	
DI-3A	10470.8	3.03		DI-3A	10470.8	3.03	
DI-3B	8782.1	5.22		DI-3B	8782.1	3.22	
EC-1A	8337.3	4.49		EC-1A	8337.3	4.49	
EC-1B	7319.9	4.58		EC-1B	7319.9	4.58	
EC-2A	9601.3	12.5		EC-2A	9800.0	12.6	
EC-2B	3708.3	5.67		EC-2B	3708.3	5.67	
EC-3A	9343.7	24.4		EC-3A	9343.7	24.4	
EC-3B	31228.4	22.1		EC-3B	31228.4	22.1	
EC-4A	20257.2	28.8		EC-4A	20257.2	28.8	
EC-4B	7978.3	7.69		EC-4B	7978.3	7.69	
LC-1A	6887.7	0.71		LC-1A	6887.7	0.71	
LC-1B	15393.8	0.964		LC-1B	15393.8	0.964	
MC-1A	10308.4	9.35		MC-1A	10308.4	9.35	
MC-1B	10640.3	2.86		MC-1B	10640.3	2.86	
MC-2A	8594.3	4.98		MC-2A	8594.3	4.98	
MC-2B	9133.8	14.2		MC-2B	9133.8	14.2	
MC-3A	5032.9	5.68		MC-3A	5032.9	5.68	
MC-3B	6018.3	18		MC-3B	6018.3	18	
PC-1A	40766.3	31.1		PC-1A	40766.3	31.1	
PC-1B	18160.8	24.5		PC-1B	18160.8	24.5	
PC-2A	3524.4	1.25		PC-2A	3524.4	1.25	
PC-2B	3473.3	1.03		PC-2B	3473.3	1.03	
PC-3A	16910.1	1.89		PC-3A	16910.1	1.89	
PC-3B	1127.6	0.694		PC-3B	1127.6	0.694	

Overall Fit	Multiple R	AIC	B-SIC	Observations
	0.472732618	27.08475404		28
R Square	0.223471212	AICc		
Adjusted R Square	0.194715985	B-SICc		
Standard Error	1.624109549			
Observations				28

ANOVA	df	SS	MS	F	p-value	sig
Regression	1	20.93379891	20.93379891	10.16251603	0.003800262	yes
Residual	26	24.88952715				
Total	27	24.88952715				

coeff	std err	tstat	p-value	lower	upper	vif
Intercept	5411.87551	993.711109	5.67111114	1.011789114	1.011789114	1
X-Aro1268(mg/kg)	205.4605044	205.059562	1.011789114	0.011789114	0.011789114	1

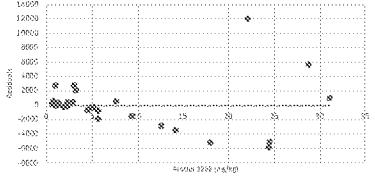
  

Location	PredY <sub>i</sub>	Res <sub>i</sub>						
DI-1A	8114.0	2.29	134.398	1340.140	2074.261752	2.3242E-07	5.32141E-07	2.1288E-05
DI-1B	8943.5	5.12	888.181	7078.455926	1.2069E-07	6.1794E-07	3.1638E-07	
DI-2A	8944.9	1.37	717.245	1812.827504	3.0425E-07	4.1689E-07	5.7110E-07	
DI-2B	6252.4	2.29	339.172	907.250000	1.3514E-07	1.3514E-07	1.3514E-07	
DI-3A	10470.8	3.03	3.375.003	1.3514E-07	2.228454741	1.1510E-07	5.805545474	5.7055055476
DI-3B	8782.1	5.22	2.700.100	1581.998	3.370.003	1.1510E-07	1.1510E-07	1.1510E-07
EC-1A	8337.3	4.49	413.869	413.869	2698.430367	1.8295E-07	5.8879795	5.8879795
EC-1B	7319.9	4.58	413.869	413.869	2698.430367	1.8295E-07	5.8879795	5.8879795
EC-2A	9601.3	12.5	12.500	12.500	2.3242E-07	2.3242E-07	2.3242E-07	2.3242E-07
EC-2B	3708.3	5.67	480.590	480.590	304.748076	3.0598E-07	3.0598E-07	3.0598E-07
EC-3A	9343.7	24.4	1868.992	1868.992	5.32141E-07	5.32141E-07	5.32141E-07	5.32141E-07
EC-3B	31228.4	22.1	17685.62	17685.62	2.3242E-07	2.3242E-07	2.3242E-07	2.3242E-07
EC-4A	20257.2	28.8	2.00E+05	2.00E+05	2.00E+05	2.00E+05	2.00E+05	2.00E+05
EC-4B	7978.3	7.69	1.00E+05	1.00E+05	1.00E+05	1.00E+05	1.00E+05	1.00E+05
LC-1A	6887.7	0.71	182.122	182.122	1026.401482	3.77117E-07	2.71901E-07	4.36914E-07
LC-1B	15393.8	0.964	946.028	946.028	1097.455577	3.47059E-07	3.47059E-07	3.47059E-07
MC-1A	10308.4							

**Case 1b: Furan Congener Concentration and Aroclor 1268 (Co-location Study Data)**

Location	Furans (mg/kg)	Aroclor 1268 (mg/kg)	Pred PCDD/F (mg/kg)	Pred PCDF/F <sup>-2</sup>	Residual PCDD/F	Residual PCDF/F <sup>-2</sup>
D1-1A	1206.0	2.29	749.82	562232.36	456.18	23939.877
D1-1B	1641.0	5.12	1889.07	3564902.53	-247.07	61042.83
D1-2A	564.5	1.37	379.79	144241.02	184.71	34117.50
D1-2B	600.4	2.29	749.82	562232.36	-149.42	2226.80
D2-1A	3831.0	3.03	1047.46	1097162.02	2783.54	7748122.64
D2-1B	3162.0	3.22	1123.87	1263993.73	2038.13	415395.85
EC-1A	999.2	4.49	1634.68	2672171.55	-635.48	40383.205
EC-1B	1001.7	4.58	1670.88	2791828.20	-669.18	4477971.16
EC-2A	2030.0	12.6	4896.58	23976493.15	2866.58	8217279.41
EC-2B	229.9	5.67	2109.28	4449072.79	-1879.38	3532078.70
EC-3A	3810.0	24.4	9642.63	9298054.24	-582.63	34019536.98
EC-3B	20737.0	22.1	8717.55	7595676.97	12019.45	144667179.73
EC-4A	17065.0	28.8	114112.34	130241491.73	5562.66	3159517.29
EC-4B	3446.0	7.66	2905.68	9462099.98	536.32	287644.25
LC-1A	728.2	0.721	118.76	1419.50	609.44	371419.36
LC-1B	2958.0	0.964	216.49	46869.89	2741.51	7515852.10
MC-1A	2089.0	9.35	3589.41	1289383.35	-1500.41	2251217.34
MC-1B	1409.0	2.86	979.08	958597.19	429.92	184831.41
MC-2A	1515.0	4.98	1831.76	3355342.62	-316.76	10036.54
MC-2B	2089.0	14.2	5540.11	30692836.13	-3451.11	11910171.02
MC-3A	1358.0	5.68	2113.39	446606.35	-755.30	570485.05
MC-3B	1872.0	18	7068.59	4996387.21	5196.59	27003608.54
PC-1A	13310.0	31.1	123374.2	15221844.57	972.58	945918.77
PC-1B	4611.0	24.5	9682.85	93757539.11	5071.35	25723638.84
PC-2A	649.3	1.24	327.50	107258.74	321.80	10355.280
PC-2B	206.7	1.93	243.04	59088.56	-36.34	1320.61
PC-3A	316.2	1.89	588.94	346848.67	-272.74	74386.34
PC-3B	206.2	0.604	71.70	5140.87	134.50	18090.28

Test for Zero Conditional Mean of Errors



No discernable relationship between residuals and independent variable  
 $\text{Cov}(\hat{u}_i, x_i) = 0$

Tests for Homoscedasticity

BREUSCH-PAGAN SUMMARY OUTPUT

Regression Statistics		$\hat{u}^2 = d_0 + d_1 x$				
Multiple R	0.523793041					
R Square	0.27437935					
Adjusted R Square	0.246644987					
Standard Error	24392362.78					
Observations	28					

$H_0$  = homoscedasticity of residuals  
 $H_a$  = heteroscedasticity of residuals  
 $p < 0.05$   
**Status: Heteroscedastic**

ANOVA

	df	SS	MS	F	Significance F
Regression	1	5.84896E+15	5.84896E+15	9.830397364	0.00426849
Residual	26	1.54697E+15	5.94587E+14		
Total	27	2.13186E+15			

Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	2557452.391	6364224.556	-0.024848089	0.699620244	-15618742.68	10503837.9	15618742.68
Aroclor 1268 (mg/kg)	1508369.505	5003845.619	3.13534645	0.004226849	540286.059	2597252.944	540286.059

WHITE'S SUMMARY OUTPUT

Regression Statistics		$\hat{u}^2 = d_0 + \hat{Y} \times d_1 Y^2 \times d_2$				
Multiple R	0.555692352					
R Square	0.303957444					
Adjusted R Square	0.25378394					
Standard Error	24273402.05					
Observations	28					

$H_0$  = homoscedasticity of residuals  
 $H_a$  = heteroscedasticity of residuals  
 $p < 0.05$   
**Status: Heteroscedastic**

ANOVA

	df	SS	MS	F	Significance F
Regression	2	6.58968E+15	3.29434E+15	5.591229002	0.009840661
Residual	25	1.4793E+15	5.89598E+14		
Total	27	2.13186E+15			

Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	770.07621	2007479.045	-0.35458238	0.349828743	-2431636651	8914244.085	2431636651
Pre PCDD/F (mg/kg)	9217.380159	4994.100051	1.87252308	0.07197753	882.8029632	19317.56328	882.8029632
Pre PCDD/F <sup>-2</sup>	-0.480432373	0.428747414	-1.120477791	0.2735159218	-1.363510427	0.402645881	0.402645881

Location	Y: Furans (mg/kg)	X: Aroclor 1268 (mg/kg)	Pred Y	Residual	Pred Resid	Weight Y	Weight X	Weight YX2
D1-1A	1206.0	2.29	749.82	456.18	805.038312	1.537304E-06	3.61083E-06	0.003214E-06
D1-1B	1641.0	5.12	1889.07	-247.07	1357.759557	5.42442E-07	2.77731E-06	1.42198E-05
D1-2A	564.5	1.37	379.79	184.71	67.41289898	2.540217E-06	3.48017E-07	4.76783E-06
D1-2B	600.4	2.29	749.82	-149.42	806.598832	1.57074E-06	3.51929E-06	8.06039E-06
D2-1A	3831.0	3.03	1047.46	2783.54	950.715802	1.19636E-06	3.35276E-06	1.01574E-05
D2-1B	3162.0	3.22	1123.87	2038.126	987.722327	1.02592E-06	3.30055E-06	1.06279E-05
EC-1A	999.2	4.49	1634.68	-635.48	125.063015	6.55573E-07	2.94353E-06	1.22164E-05
EC-1B	1001.7	4.58	1670.88	-669.18	1252.591058	6.37255E-07	2.91909E-06	1.23694E-05
EC-2A	2030.0	12.6	4898.58	2866.59	2814.527802	1.26327E-07	1.59059E-06	2.08413E-05
EC-2B	229.9	5.67	2109.28	-1979.29	1464.875622	4.66103E-07	2.66222E-06	1.49819E-05
EC-3A	3810.0	24.4	9642.63	-5832.67	512.663877	3.32585E-08	9.33459E-07	2.27764E-05
EC-3B	20737.0	22.1	8717.55	1209.450	4664.724049	4.59566E-09	1.01564E-06	2.24547E-05
EC-4A	17065.0	28.8	1141.234	1019.45	4664.872404	8.08171E-07	2.32753E-05	
EC-4B	3446.0	7.66	2905.68	536.325	1852.44052	2.91415E-07	2.23224E-06	1.70898E-05
LC-1A	728.2	0.721	118.76	609.44	501.0259656	3.98363E-06	2.07096E-06	
LC-1B	2958.0	0.964	216.49	2741.505	543.3517823	3.32596E-06	3.20596E-06	3.09055E-06
EC-2A	206.2	1.24	327.50	321.796	602.1045617	2.75833E-06	3.42041E-06	4.24131E-06
PC-1A	13310.0	31.1	123374.2	972.584	647.1532073	2.42809E-08	7.55134E-07	2.34847E-05
PC-1B	4611.0	24.5	9682.85	5071.85	5132.139522	3.79667E-08	9.30185E-07	2.27895E-05
PC-2A	649.3	1.24	327.50	321.796	561.2057078	3.17059E-06	3.27034E-06	3.36845E-06
PC-2B	206.7	1.03	243.04	-36.34	561.2057078	3.17059E-06	3.27034E-06	3.36845E-06
PC-3A	316.2	1.89	588.94	272.739	728.6962523	1.88325E-06	3.55933E-06	6.77214E-06
PC-3B	206.2	0.604	71.70	134.500	478.2394613	4.37229E-06	2.64086E-06	1.59503E-06

SUM  $\sum W_i$  3.27343E-05  $\sum W_i^2$  6.91609E-05  $\sum W_i W_i^2$  0.000369863

Var  $= \frac{\sum W_i}{(\sum W_i)(\sum W_i^2) - (\sum W_i^2)^2}$

Error Variance of OLS

4469

Case 1b: Furan Congener Concentration and Aroclor 1268 (Co-location Study Data)

Iteration	Iteration [mg/kg]	Aroclor 1268 [mg/kg]
01-1A	1206.0	2.29
01-1B	1641.0	5.12
01-2A	964.5	1.37
01-2B	600.4	2.29
02-1A	2831.0	3.03
02-1B	3162.0	3.22
EC-1A	995.2	4.49
EC-1B	1001.7	4.58
EC-2A	265.0	1.25
EC-2B	229.9	5.67
EC-3A	3810.0	24.4
EC-3B	20737.0	22.1
EC-4A	1705.0	28.8
EC-4B	3446.0	7.68
LC-1A	728.2	0.71
LC-1B	2958.0	0.964
MC-1A	2099.0	9.35
MC-1B	1409.0	2.88
MC-2A	1515.0	4.98
MC-2B	2609.0	14.2
MC-3A	1238.0	5.68
MC-3B	1872.0	18
PC-1A	13110.0	31.3
PC-1B	4611.0	24.5
PC-2A	643.3	1.25
PC-2B	205.7	1.03
PC-3A	316.2	1.89
PC-3B	205.2	0.694

Iteration #1	X-Aroclor 1268 [mg/kg]	X-Aroclor 1268 [mg/kg]	Pred Y <sub>i</sub>	Residual [mg/kg]	Aroclor 1268 [mg/kg]	Pred Y <sub>i</sub>	Residual [mg/kg]	Aroclor 1268 [mg/kg]	Pred Y <sub>i</sub>	Residual [mg/kg]	Aroclor 1268 [mg/kg]
01-1A	1206.0	2.29	1.75E+02	-4.56E+02	4.56E+02	8.07E+02	1.54E+03	8.07E+02	1.54E+03	8.07E+02	1.54E+03
01-1B	1641.0	5.12	1.89E+03	-2.47E+02	2.47E+02	1.93E+03	5.42E+02	1.93E+03	5.42E+02	1.93E+03	5.42E+02
01-2A	964.5	1.37	3.80E+02	-1.85E+02	1.85E+02	6.27E+02	2.94E+02	6.27E+02	2.94E+02	6.27E+02	2.94E+02
01-2B	600.4	2.29	7.50E+02	-1.42E+02	1.42E+02	8.07E+02	1.05E+03	8.07E+02	1.05E+03	8.07E+02	1.05E+03
02-1A	2831.0	3.03	1.08E+03	-2.78E+02	2.78E+02	9.51E+02	2.11E+03	9.51E+02	2.11E+03	9.51E+02	2.11E+03
02-1B	3162.0	5.22	1.12E+03	-2.04E+03	2.04E+03	9.88E+02	1.03E+03	9.88E+02	1.03E+03	9.88E+02	1.03E+03
EC-1A	995.2	4.49	1.63E+03	-6.35E+02	6.35E+02	1.24E+03	6.56E+02	1.24E+03	6.56E+02	1.24E+03	6.56E+02
EC-1B	1001.7	4.58	1.67E+03	-6.89E+02	6.89E+02	1.25E+03	6.37E+02	1.25E+03	6.37E+02	1.25E+03	6.37E+02
EC-2A	2036.0	12.5	4.90E+03	-2.87E+03	2.87E+03	2.81E+03	1.26E+02	2.81E+03	1.26E+02	2.81E+03	1.26E+02
EC-2B	223.9	5.67	2.11E+03	-3.89E+02	3.89E+02	1.34E+03	4.09E+02	1.34E+03	4.09E+02	1.34E+03	4.09E+02
EC-3A	3810.0	24.4	9.64E+03	-5.83E+03	5.83E+03	5.11E+03	3.83E+03	5.11E+03	3.83E+03	5.11E+03	3.83E+03
EC-3B	20737.0	22.1	3.87E+03	-1.20E+04	1.20E+04	4.65E+03	4.60E+03	4.65E+03	4.60E+03	4.65E+03	4.60E+03
EC-4A	1705.0	28.8	1.14E+04	5.65E+03	5.65E+03	5.97E+03	2.81E+03	5.97E+03	2.81E+03	5.97E+03	2.81E+03
EC-4B	3446.0	7.68	3.91E+03	-5.36E+02	5.36E+02	1.85E+03	2.91E+03	1.85E+03	2.91E+03	1.85E+03	2.91E+03
LC-1A	728.2	0.71	1.01E+03	-6.06E+02	6.06E+02	1.25E+02	8.29E+02	1.25E+02	8.29E+02	1.25E+02	8.29E+02
LC-1B	2958.0	0.964	2.15E+02	-2.74E+03	2.74E+03	5.48E+02	3.33E+03	5.48E+02	3.33E+03	5.48E+02	3.33E+03
MC-1A	2099.0	9.35	3.59E+03	-1.50E+03	1.50E+03	2.18E+03	2.10E+03	2.18E+03	2.10E+03	2.18E+03	2.10E+03
MC-1B	1409.0	2.88	1.80E+03	-1.50E+03	1.50E+03	2.10E+03	1.50E+03	2.10E+03	1.50E+03	2.10E+03	1.50E+03
MC-2A	1515.0	4.98	1.83E+03	-3.17E+02	3.17E+02	1.33E+03	5.65E+02	1.33E+03	5.65E+02	1.33E+03	5.65E+02
MC-2B	2609.0	14.2	5.23E+03	-3.95E+02	3.95E+02	1.91E+02	4.30E+02	1.91E+02	4.30E+02	1.91E+02	4.30E+02
MC-3A	1238.0	5.68	2.11E+03	-2.55E+02	2.55E+02	1.47E+03	4.65E+02	1.47E+03	4.65E+02	1.47E+03	4.65E+02
MC-3B	1872.0	19	7.07E+03	-5.20E+03	5.20E+03	1.87E+03	6.69E+03	1.87E+03	6.69E+03	1.87E+03	6.69E+03
PC-1A	13110.0	31.1	1.21E+04	9.73E+02	9.73E+02	6.42E+03	2.41E+03	6.42E+03	2.41E+03	6.42E+03	2.41E+03
PC-1B	4611.0	24.5	9.68E+03	-5.07E+03	5.07E+03	5.13E+03	2.52E+03	5.13E+03	2.52E+03	5.13E+03	2.52E+03
PC-2A	643.3	1.25	3.28E+03	-2.87E+02	2.87E+02	1.25E+03	2.02E+02	1.25E+03	2.02E+02	1.25E+03	2.02E+02
PC-2B	205.7	1.03	1.04E+02	-2.53E+02	2.53E+02	6.01E+02	1.18E+03	6.01E+02	1.18E+03	6.01E+02	1.18E+03
PC-3A	316.2	1.89	1.10E+02	-7.83E+02	7.83E+02	6.73E+02	1.08E+03	6.73E+02	1.08E+03	6.73E+02	1.08E+03
PC-3B	206.2	0.694	7.17E+01	-1.35E+02	1.35E+02	4.78E+02	4.37E+03	4.78E+02	4.37E+03	4.78E+02	4.37E+03

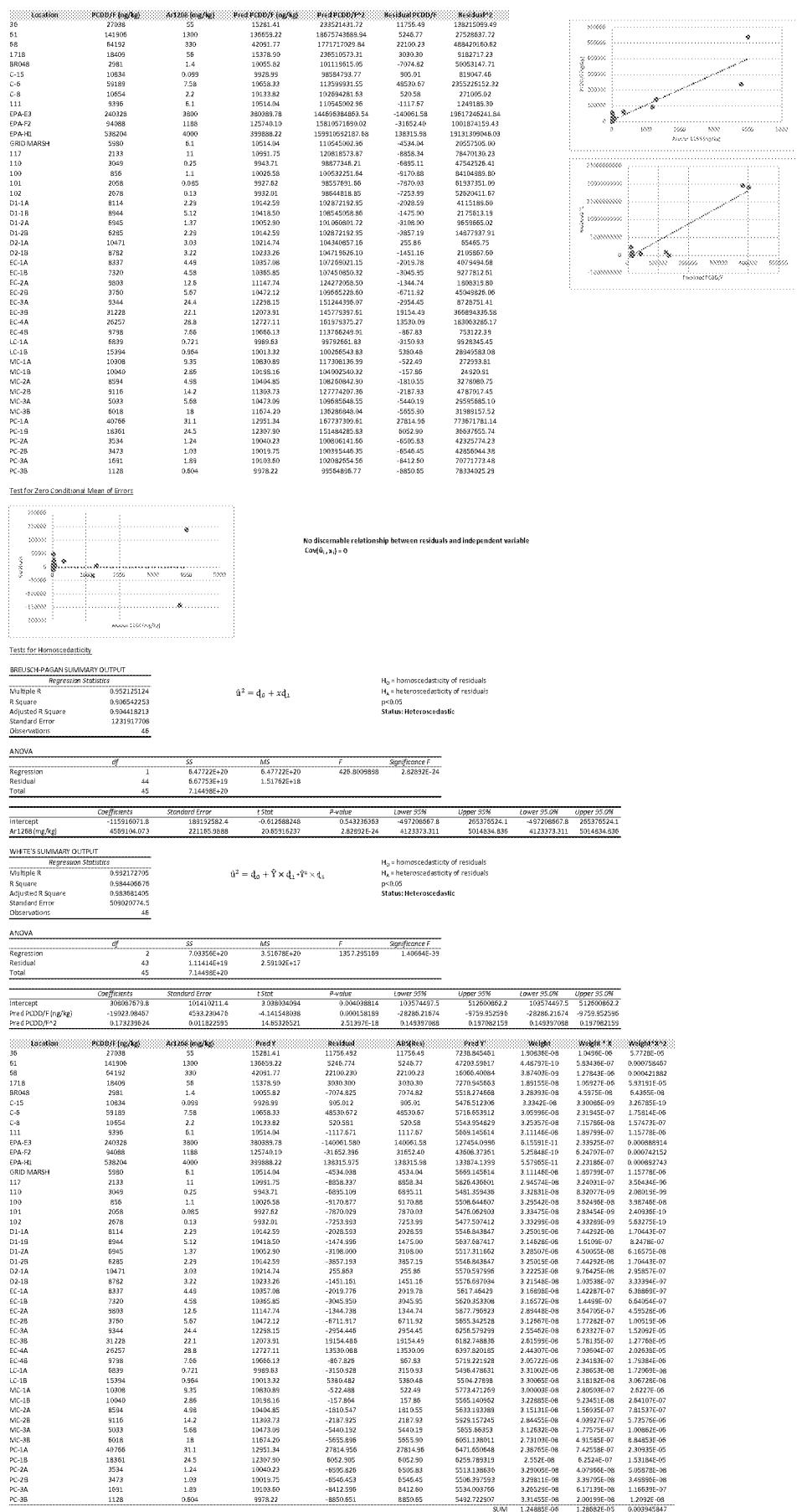
  

Iteration #2	X-Aroclor 1268 [mg/kg]	X-Aroclor 1268 [mg/kg]	Pred Y <sub>i</sub>	Residual [mg/kg]	Aroclor 1268 [mg/kg]	Pred Y <sub>i</sub>	Residual [mg/kg]	Aroclor 1268 [mg/kg]	Pred Y <sub>i</sub>	Residual [mg/kg]	Aroclor 1268 [mg/kg]
01-1A	1206.0	2.29	7.31E+02	-6.60E+02	6.60E+02	2.30E+02	4.09E+02	2.30E+02	4.09E+02	2.30E+02	4.09E+02
01-1B	1641.0	5.12	1.95E+03	-2.47E+02	2.47E+02	1.54E+03	5.42E+02	1.54E+03	5.42E+02	1.54E+03	5.42E+02
01-2A	964.5	1.37	9.51E+02	-3.87E+02	3.87E+02	4.59E+02	4.74E+02	4.59E+02	4.74E+02	4.59E+02	4.74E+02
01-2B	600.4	2.29	1.21E+03	-4.15E+02	4.15E+02	6.15E+02	2.70E+02	6.15E+02	2.70E+02	6.15E+02	2.70E+02
02-1A	2831.0	3.03	1.42E+03	-2.41E+03	2.41E+03	8.12E+02	1.49E+03	8.12E+02	1.49E+03	8.12E+02	1.49E+03
02-1B	3162.0	5.22	1.49E+03	-1.08E+03	1.08E+03	8.63E+02	1.34E+03	8.63E+02	1.34E+03	8.63E+02	1.34E+03
EC-1A	995.2	4.49	1.84E+03	-8.41E+02	8.41E+02	7.11E+02	7.71E+02	7.11E+02	7.71E+02	7.11E+02	7.71E+02
EC-1B	1001.7	4.58	1.87E+03	-8.85E+02	8.85E+02	7.15E+02	7.45E+02	7.15E+02	7.45E+02	7.15E+02	7.45E+02
EC-2A	265.0	1.25	4.15E+02	-4.15E+02	4.15E+02	2.50E+02	1.65E+02	2.50E+02	1.65E+02	2.50E+02	1.65E+02
EC-2B	229.9	5.67	2.15E+03	-1.95E+03	1.95E+03	1.40E+03	5.13E+03	1.40E+03	5.13E+03	1.40E+03	5.13E+03
EC-3A	3810.0	26.4	7.52E+03	-3.71E+03	3.71E+03	5.13E+03	5.34E+03	5.13E+03	5.34E+03	5.13E+03	5.34E+03
EC-3B	20737.0	22.1	8.77E+03	-1.20E+04	1.20E+04	8.46E+03	2.41E+03	8.46E+03	2.41E+03	8.46E+03	2.41E+03
EC-4A	1705.0	28.8	8.29E+03	-8.29E+02	8.29E+02	7.25E+03	1.24E+03	7.25E+03	1.24E+03	7.25E+03	1.24E+03
EC-4B	3446.0	7.68	3.28E+03	-2.95E+02	2.95E+02	2.52E+03	3.04E+02	2.52E+03	3.04E+02	2.52E+03	3.04E+02
LC-1A	728.2	0.71	7.67E+02	-3.78E+03	3.78E+03	7.15E+02	8.88E+02	7.15E+02	8.88E+02	7.15E+02	8.88E+02
LC-1B	2958.0	0.964	2.12E+03	-2.12E+03	2.12E+03	3.71E+02	7.26E+03	3.71E+02	7.26E+03	3.71E+02	7.26E+03
MC-1A	2099.0	9.35	3.23E+03	-1.14E+03	1.14E+03	2.02E+03	7.07E+03	2.02E+03	7.07E+03	2.02E+03	7.07E+03
MC-1B	1409.0	2.88	1.38E+03	-1.38E+03	1.38E+03	6.00E+02	1.03E+03	6.00E+02	1.03E+03	6.00E+02	1.03E+03
MC-2A	1515.0	4.98	1.83E+03	-3.23E+02	3.23E+02	5.44E+03	9.00E+02	5.44E+03	9.00E+02	5.44E+03	9.00E+02
MC-2B	2609.0	14.2	6.01E+03	-2.52E+02	2.52E+02	6.00E+03	6.00E+02	6.00E+03	6.00E+02	6.00E+03	6.00E+02
MC-3A	1238.0	5.68	2.18E+03	-8.29E+02	8.29E+02	1.40E+03	5.11E+03	1.40E+03	5.11E+03	1.40E+03	5.11E+03
MC-3B	1872.0	19	5.69E+03	-3.92E+03	3.92E+03	6.00E+03	6.00E+03	6.00E+03	6.00E+03	6.00E+03	6.00E+03
PC-1A	13110.0	31.1	9.43E+03	-3.86E+03	3.86E+03	6.94E+03	2.08E+03	6.94E+03	2.08E+03	6.94E+03	2.08E+03
PC-1B	4611.0	24.5	9.83E+03	-2.65E+02	2.65E+02	4.21E+03	2.42E+03	4.21E+03	2.42E+03	4.21E+03	2.42E+03
PC-2A	643.3	1.25	3.13E+03	-2.55E+02	2.55E+02	3.25E+02	4.20E+02	3.25E+02	4.20E+02	3.25E+02	4.20E+02
PC-2B	205.7	1.03	1.04E+02	-2.53E+02	2.53E+02	6.01E+02	3.01E+03	6.01E+02	3.01E+03	6.01E+02	3.01E+03
PC-3A	316.2	1.89	1.10E+02	-7.83E+02	7.83E+02	6.73E+02	7.37E+02	6.73E+02	7.37E+02	6.73E+02	7.37E+02
PC-3B	206.2	0.694	7.32E+02	-5.26E+02	5.26E+02	3.26E+02	1.17E+03	3.26E+02	1.17E+03	3.26E+02	1.17E+03

Iteration #3	X-Aroclor 1268 [mg/kg]	X-Aroclor 1268 [mg/kg]	Pred Y <sub>i</sub>	Residual [mg/kg]	Aroclor 1268 [mg/kg]	Pred Y <sub>i</sub>	Residual [mg/kg]	Aroclor 1268 [mg/kg]	Pred Y <sub>i</sub>	Residual [mg/kg]	Aroclor 1268 [mg/kg]
01-1A	12										

**Case 2a: PCDD/F Concentration and Aroclor 1268 (Cumulative Data Set)**





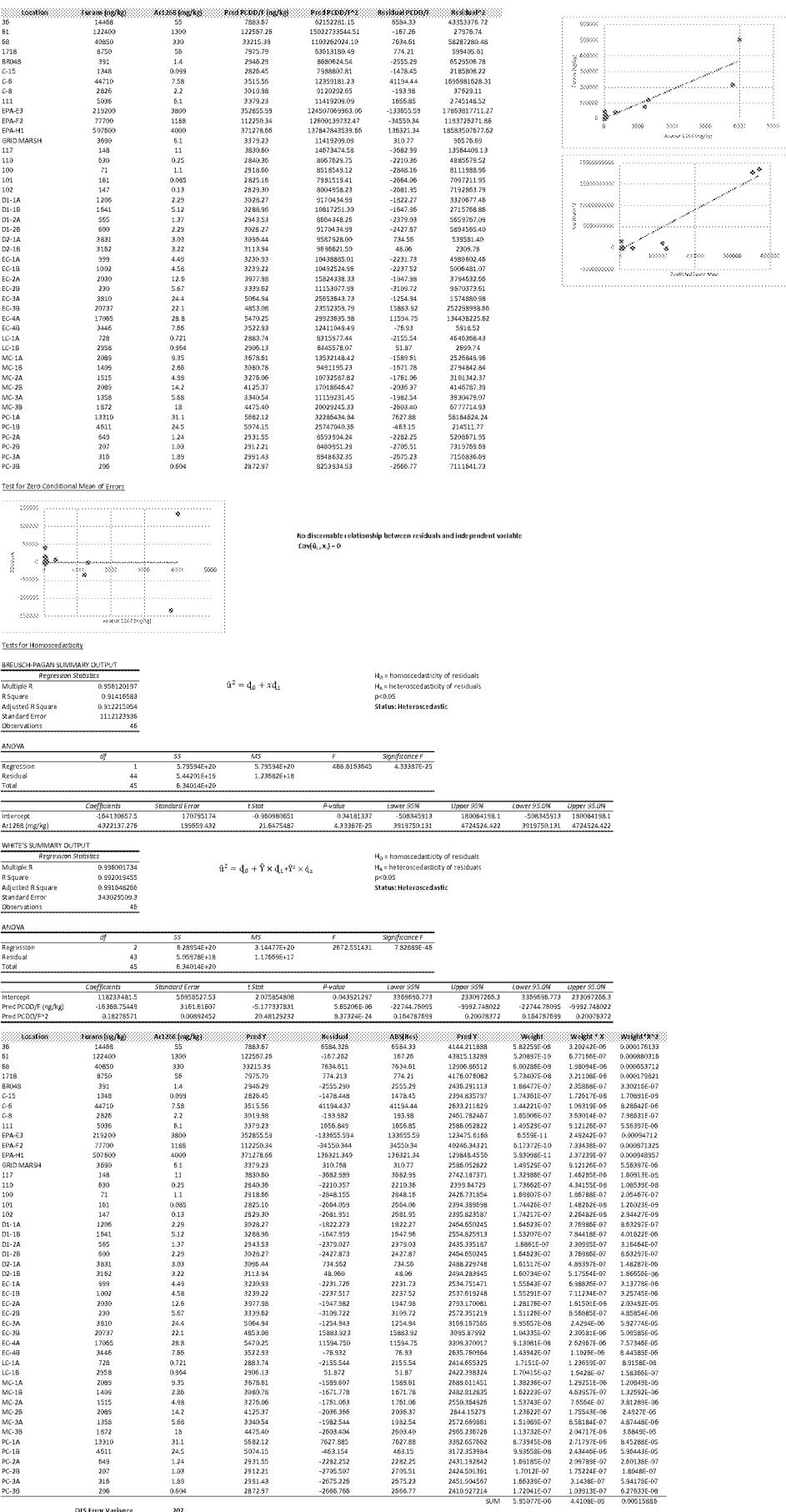
**Case 2a: PCDD/F Concentration and Aroclor 1268 (Cumulative Data Set)**

Location	PCDD/F (ng/kg)	Aroclor 1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight	Weight * X	Weight*X^2
36	27038	55	15717.93	11319.972	11319.97	7470.494248	1.79185E-08	9.85517E-07	5.42034E-05
61	141906	1300	158882.57	-16976.567	16976.57	47727.38638	4.39E-10	5.707E-07	0.00074191
68	64192	330	47340.64	16851.360	16851.36	16362.57886	3.73505E-09	1.23257E-06	0.000406747
1718	18409	56	15832.92	2576.281	2576.28	7502.829101	1.77644E-08	9.94805E-07	5.57091E-05
BR048	2981	1.4	9554.37	-6573.374	6573.37	5737.34612	3.03793E-08	4.2531E-08	5.95434E-08
C-15	10834	0.099	9404.77	1429.230	1429.23	5695.278477	3.08298E-08	3.05215E-09	3.02162E-10
C-6	59189	7.58	10265.02	48923.977	48923.98	5937.175513	2.83688E-08	2.15035E-07	1.62997E-06
C-8	10654	2.2	9646.37	1008.033	1008.03	5763.214003	3.01072E-08	6.62359E-08	1.45719E-07
111	9396	6.1	10094.83	-698.468	698.47	5889.31993	2.88317E-08	1.75873E-07	1.07283E-06
EPA-E3	240328	3800	446361.76	-206033.557	206033.56	128564.5192	6.05003E-11	2.29901E-07	0.000873625
EPA-F2	94088	1188	146003.50	-51915.797	51915.80	44105.88283	5.14052E-10	6.10694E-07	0.000725504
EPA-H1	538204	4000	469360.09	68844.108	68844.11	135031.4898	5.48441E-11	2.19376E-07	0.000877506
GRID MARSH	5980	6.1	10094.83	-4114.835	4114.83	5889.31993	2.88317E-08	1.75873E-07	1.07283E-06
117	2133	11	10658.29	-8524.880	8524.88	6047.76071	2.73408E-08	3.00749E-07	3.30823E-06
110	3049	0.25	9422.13	-6373.533	6373.53	5700.161039	3.0777E-08	7.69424E-09	1.92356E-09
100	856	1.1	9519.88	-8664.176	8664.18	5727.645665	3.04823E-08	3.35305E-08	3.68836E-08
101	2058	0.085	9403.16	-7345.566	7345.57	5694.825789	3.08347E-08	2.62095E-09	2.2278E-10
102	2678	0.13	9408.33	-6730.317	6730.32	5696.280857	3.08189E-08	4.00646E-09	5.2084E-10
D1-1A	8114	2.29	9656.72	-1542.716	1542.72	5766.12414	3.00768E-08	6.88759E-08	1.57726E-07
D1-1B	8944	5.12	9982.14	-1038.643	1038.64	5857.631774	2.91445E-08	1.4922E-07	7.64004E-07
D1-2A	6945	1.37	9550.92	-2606.024	2606.02	5736.376075	3.03896E-08	4.16337E-08	5.70382E-08
D1-2B	6285	2.29	9656.72	-3371.316	3371.32	5766.12414	3.00768E-08	6.88759E-08	1.57726E-07
D2-1A	10471	3.03	9741.81	728.790	728.79	5790.051931	2.98288E-08	9.03811E-08	2.73855E-07
D2-1B	8782	3.22	9763.66	-981.559	981.56	5796.195553	2.97656E-08	9.58451E-08	3.08621E-07
EC-1A	8337	4.49	9909.70	-1572.398	1572.40	5837.260817	2.93482E-08	1.31774E-07	5.91663E-07
EC-1B	7320	4.58	9920.05	-2600.147	2600.15	5840.170953	2.9319E-08	1.34281E-07	6.15007E-07
EC-2A	9803	12.6	10842.28	-1039.281	1039.28	6099.496475	2.68789E-08	3.38675E-07	4.2673E-06
EC-2B	3760	5.67	10045.39	-6285.188	6285.19	5875.415943	2.89683E-08	1.6425E-07	9.31298E-07
EC-3A	9344	24.4	12199.18	-2855.482	2855.48	6481.047742	2.38073E-08	5.80897E-07	1.41739E-05
EC-3B	31228	22.1	11934.70	19293.698	19293.70	6406.67758	2.43632E-08	5.38427E-07	1.18992E-05
EC-4A	26257	28.8	12705.15	13552.054	13552.05	6623.321096	2.27955E-08	6.56509E-07	1.89075E-05
EC-4B	9798	7.66	10274.22	-475.922	475.92	5939.762301	2.8344E-08	2.17115E-07	1.6631E-06
LC-1A	6839	0.721	9476.29	-2637.594	2637.59	5715.390755	3.06132E-08	2.20721E-08	1.5914E-08
LC-1B	15394	0.964	9504.24	5889.563	5889.56	5723.248125	3.05292E-08	2.94301E-08	2.83706E-08
MC-1A	10308	9.35	10468.56	-160.158	160.16	5994.408203	2.78296E-08	2.60207E-07	2.43294E-06
MC-1B	10040	2.86	9722.26	318.038	318.04	5784.555006	2.98855E-08	8.54724E-08	2.44451E-07
MC-2A	8594	4.98	9966.04	-1371.744	1371.74	5853.104895	2.91895E-08	1.45364E-07	7.23912E-07
MC-2B	9116	14.2	11026.27	-1910.467	1910.47	6151.23224	2.64287E-08	3.75287E-07	5.32908E-06
MC-3A	5033	5.68	10046.54	-5013.638	5013.64	5875.739292	2.89651E-08	1.64522E-07	9.34483E-07
MC-3B	6018	18	11463.24	-5444.936	5444.94	6274.104682	2.54037E-08	4.57266E-07	8.23079E-06
PC-1A	40766	31.1	12969.63	27796.673	27796.67	6697.691258	2.2292E-08	6.93282E-07	2.15611E-05
PC-1B	18361	24.5	12210.68	6150.118	6150.12	6484.281228	2.37835E-08	5.82696E-07	1.42761E-05
PC-2A	3534	1.24	9535.98	-6001.575	6001.58	5732.172544	3.04342E-08	3.77384E-08	4.67956E-08
PC-2B	3473	1.03	9511.83	-6038.527	6038.53	5725.382225	3.05064E-08	3.14216E-08	3.23642E-08
PC-3A	1691	1.89	9610.72	-7919.720	7919.72	5753.190198	3.02122E-08	5.71011E-08	1.07921E-07
PC-3B	1128	0.604	9462.84	-8335.270	8335.27	5711.607577	3.06537E-08	1.85149E-08	1.1183E-08
SUM								1.15792E-06	1.21079E-05
WLS Error Variance								0.003851276	

$$Var = \frac{\sum w_i}{((\sum w_i)(\sum w_i x_i^2) - (\sum w_i x_i)^2)}$$

WLS Var:OLS Var = 1.02  
Heteroscedasticity not severe

Case 2b: Furam Congener Concentration and Aroclor 1268 (Cumulative Data Set)



Case 2b: Furam Congener Concentration and Aroclor 1268 (Cumulative Data Set)

Iteration #2

	Sample ID	Conc (ng/g)	Aroclor 1268 (Cumulative)
36	14488	55	
61	129400	1300	
68	40800	350	
1718	8750	56	
BR0048	391	1.4	
C-13	1348	0.99	
C-6	47410	7.58	
C-5	3826	2.2	
111	2651	6.1	
BR0049	226000	16000	
EPA#2	77700	1188	
EPA#13	507600	4000	
G40/MARSH	51650	6.1	
121	1348	1.1	
130	880	0.25	
200	71	1.1	
101	130	0.98	
102	147	0.13	
O1-1A	1208	2.29	
O1-1B	1641	9.12	
O1-2A	1505	1.77	
O1-2B	148	4.49	
EC-1B	1020	4.58	
EC-2A	2020	12.6	
EC-2B	1293	5.87	
EC-3A	5810	34.4	
EC-3B	26797	22.1	
EC-4A	1748	2.68	
EC-4B	1448	7.66	
LC-1A	728	0.721	
LC-1B	2584	0.954	
MC-2A	286	9.35	
MC-2B	1409	2.86	
MC-2C	1515	4.98	
MC-2D	2000	14.2	
MC-5A	1598	9.68	
MC-5B	187	1.68	
PC-10	19150	91.1	
PC-19	6401	24.5	
PC-2A	649	1.24	
PC-13A	218	1.08	
PC-13B	318	1.89	
PC-19B	508	0.604	

Weighted Least Squares performed with "Real Stats" Add-in

Pred  $Y'$  = Abs(Res)x +  $\delta_1$ 

$$W_i = \frac{1}{Pred Y_i^2}$$

WLS solution is asymptotic at iteration #4.

Iteration #3

	Sample ID	Conc (ng/g)	Aroclor 1268 (Cumulative)
36	14488	55	7.58E+00
61	129400	1300	1.23E+00
68	40800	350	1.67E+00
1718	8750	56	1.98E+00
BR0048	391	1.4	2.59E+00
C-15	0.09	2.88E+00	3.12E+00
C-6	47410	7.58	4.12E+00
C-5	3826	2.2	5.06E+00
111	2651	6.1	5.88E+00
BR0049	226000	16000	1.34E+00
EPA#2	77700	1188	1.21E+00
EPA#13	507600	4000	9.46E+00
G40/MARSH	51650	6.1	1.11E+00
121	1348	1.1	1.18E+00
130	880	0.25	1.25E+00
200	71	1.1	1.29E+00
101	130	0.98	1.32E+00
102	147	0.13	1.35E+00
O1-1A	1208	2.29	1.38E+00
O1-1B	1641	9.12	1.41E+00
O1-2A	1505	1.77	1.44E+00
O1-2B	148	4.49	1.48E+00
EC-1B	1020	4.58	1.51E+00
EC-2A	2020	12.6	1.54E+00
EC-2B	1293	5.87	1.57E+00
EC-3A	5810	34.4	1.59E+00
EC-3B	26797	22.1	1.62E+00
EC-4A	1748	2.68	1.65E+00
EC-4B	1448	7.66	1.68E+00
LC-1A	728	0.721	1.72E+00
LC-1B	2584	0.954	1.75E+00
MC-2A	286	9.35	1.78E+00
MC-2B	1409	2.86	1.80E+00
MC-2C	1515	4.98	1.82E+00
MC-2D	2000	14.2	1.84E+00
MC-5A	1598	9.68	1.86E+00
MC-5B	187	1.68	1.88E+00
PC-10	19150	91.1	1.90E+00
PC-19	6401	24.5	1.93E+00
PC-2A	649	1.24	1.95E+00
PC-13A	218	1.08	1.97E+00
PC-13B	318	1.89	1.99E+00
PC-19B	508	0.604	2.01E+00

Iteration #3

	Sample ID	Conc (ng/g)	Aroclor 1268 (Cumulative)
36	14488	55	7.58E+00
61	129400	1300	1.23E+00
68	40800	350	1.67E+00
1718	8750	56	1.98E+00
BR0048	391	1.4	2.59E+00
C-15	0.09	2.88E+00	3.12E+00
C-6	47410	7.58	4.12E+00
C-5	3826	2.2	5.06E+00
111	2651	6.1	5.88E+00
BR0049	226000	16000	1.34E+00
EPA#2	77700	1188	1.21E+00
EPA#13	507600	4000	9.46E+00
G40/MARSH	51650	6.1	1.11E+00
121	1348	1.1	1.18E+00
130	880	0.25	1.25E+00
200	71	1.1	1.29E+00
101	130	0.98	1.32E+00
102	147	0.13	1.35E+00
O1-1A	1208	2.29	1.38E+00
O1-1B	1641	9.12	1.41E+00
O1-2A	1505	1.77	1.44E+00
O1-2B	148	4.49	1.48E+00
EC-1B	1020	4.58	1.51E+00
EC-2A	2020	12.6	1.54E+00
EC-2B	1293	5.87	1.57E+00
EC-3A	5810	34.4	1.59E+00
EC-3B	26797	22.1	1.62E+00
EC-4A	1748	2.68	1.65E+00
EC-4B	1448	7.66	1.68E+00
LC-1A	728	0.721	1.72E+00
LC-1B	2584	0.954	1.75E+00
MC-2A	286	9.35	1.78E+00
MC-2B	1409	2.86	1.80E+00
MC-2C	1515	4.98	1.82E+00
MC-2D	2000	14.2	1.84E+00
MC-5A	1598	9.68	1.86E+00
MC-5B	187	1.68	1.88E+00
PC-10	19150	91.1	1.90E+00
PC-19	6401	24.5	1.93E+00
PC-2A	649	1.24	1.95E+00
PC-13A	218	1.08	1.97E+00
PC-13B	318	1.89	1.99E+00
PC-19B	508	0.604	2.01E+00

Iteration #4

	Sample ID	Conc (ng/g)	Aroclor 1268 (Cumulative)
36	14488	55	7.58E+00
61	129400	1300	1.23E+00
68	40800	350	1.67E+00
1718	8750	56	1.98E+00
BR0048	391	1.4	2.59E+00
C-15	0.09	2.88E+00	3.12E+00
C-6	47410	7.58	4.12E+00
C-5	3826	2.2	5.06E+00
111	2651	6.1	5.88E+00
BR0049	226000	16000	1.34E+00
EPA#2	77700	1188	1.21E+00
EPA#13	507600	4000	9.46E+00
G40/MARSH	51650	6.1	1.11E+00
121	1348	1.1	1.18E+00
130	880	0.25	1.25E+00
200	71	1.1	1.29E+00
101	130	0.98	1.32E+00
102	147	0.13	1.35E+00
O1-1A	1208	2.29	1.38E+00
O1-1B	1641	9.12	1.41E+00
O1-2A	1505	1.77	1.44E+00
O1-2B	148	4.49	1.48E+00
EC-1B	1020	4.58	1.51E+00
EC-2A	2020	12.6	1.54E+00
EC-2B	1293	5.87	1.57E+00
EC-3A	5810	34.4	1.59E+00
EC-3B	26797	22.1	1.62E+00
EC-4A	1748	2.68	1.65E+00
EC-4B	1448	7.66	1.68E+00
LC-1A	728	0.721	1.72E+00
LC-1B	2584	0.954	1.75E+00
MC-2A	286	9.35	1.78E+00
MC-2B	1409	2.86	1.80E+00
MC-2C	1515	4.98	1.82E+00
MC-2D	2000	14.2	1.84E+00
MC-5A	1598	9.68	1.86E+00
MC-5B	187	1.68	1.88E+00
PC-10	19150	91.1	1.90E+00
PC-19	6401	24.5	1.93E+00
PC-2A	649	1.24	1.95E+00
PC-13A	218	1.08	1.97E+00
PC-13B	318	1.89	1.99E+00
PC-19B	508	0.604	2.01E+00

Iteration #5

	Sample ID	Conc (ng/g)	Aroclor 1268 (Cumulative)
36	14488	55	7.58E+00
61	129400	1300	1.23E+00
68	40800	350	1.67E+00
1718	8750	56	1.98E+00
BR0048	391	1.4	2.59E+00
C-15	0.09	2.88E+00	3.12E+00
C-6	47410	7.58	4.12E+00
C-5	3826	2.2	5.06E+00
111	2651	6.1	5.88E+00
BR0049	226000	16000	1.34E+00
EPA#2	77700	1188	1.21E+00
EPA#13	507600	4000	9.46E+00
G40/MARSH	51650	6.1	1.11E+00
121	1348	1.1	1.18E+00
130	880	0.25	1.25E+00
200	71	1.1	1.29E+00
101	130	0.98	1.32E+00
102	147	0.13	1.35E+00
O1-1A	1208	2.29	1.38E+00
O1-1B	1641	9.12	1.41E+00
O1-2A	1505	1.77	1.44E+00
O1-2B	148	4.49	1.48E+00
EC-1B	1020	4.58	1.51E+00
EC-2A	2020	12.6	1.54E+00
EC-2B	1293	5.87	1.57E+00
EC-3A	5810	34.4	1.59E+00
EC-3B	26797	22.1	1.62E+00
EC-4A	1748	2.68	1.65E+00
EC-4B	1448	7.66	1.68E+00
LC-1A	728	0.721	1.72E+00
LC-1B	2584	0.954	1.75E+00
MC-2A	286	9.35	1.78E+00
MC-2B	1409	2.86	1.80E+00
MC-2C	1515	4.98	1.82E+00
MC-2D	2000	14.2	1.84E+00
MC-5A	1598	9.68	1.86E+00
MC-5B	187	1.68	1.88E+00
PC-10	19150	91.1	1.90E+00
PC-19	6401	24.5	1.93E+00
PC-2A	649	1.24	1.95E+00
PC-13A	218	1.08	1.97E+00
PC-13B	318	1.89	1.99E+00
PC-19B	508	0.604	2.01E+00

Iteration #6

	Sample ID	Conc (ng/g)	Aroclor 1268 (Cumulative)
36	1448		

**Case 2b: Furan Congener Concentration and Aroclor 1268 (Cumulative Data Set)**

Location	Furans (ng/kg)	Aroclor 1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight	Weight * X	Weight*X^2
36	14468	55	8773.22	5694.780	5694.78	4723.682393	4.48166E-08	2.46491E-06	0.00013557
61	122400	1300	142854.02	-20454.021	20454.02	44994.11531	4.93956E-10	6.42143E-07	0.000834786
68	40850	330	38389.46	2460.539	2460.54	13618.75794	5.39169E-09	1.77926E-06	0.000587155
1718	8750	56	8880.91	-130.915	130.91	4756.028122	4.4209E-08	2.47571E-06	0.00013864
BR048	391	1.4	3000.74	-2609.745	2609.74	2989.951306	1.11859E-07	1.56603E-07	2.19244E-07
C-15	1348	0.099	2860.63	-1512.633	1512.63	2947.869512	1.15076E-07	1.13925E-08	1.12786E-09
C-6	44710	7.58	3666.30	41043.697	41043.70	3189.847912	9.82788E-08	7.44954E-07	5.64675E-06
C-8	2826	2.2	3086.90	-260.901	260.90	3015.827889	1.09948E-07	2.41885E-07	5.32148E-07
111	5036	6.1	3506.91	1529.168	1529.17	3141.976233	1.01296E-07	6.17908E-07	3.76924E-06
EPA-E3	219200	3800	412092.58	-192892.575	192892.58	125858.4384	6.31299E-11	2.39894E-07	0.000911596
EPA-F2	77700	1188	130792.13	-53092.133	53092.13	41371.39363	5.84251E-10	6.94091E-07	0.00082458
EPA-H1	507600	4000	433631.66	73968.340	73968.34	132327.5843	5.71083E-11	2.28433E-07	0.000913733
GRID MARSH	3690	6.1	3506.91	183.087	183.09	3141.976233	1.01296E-07	6.17908E-07	3.76924E-06
117	148	11	4034.62	-3887.013	3887.01	3300.470306	9.18012E-08	1.00981E-06	1.11079E-05
110	630	0.25	2876.90	-2246.895	2246.90	2952.753717	1.14695E-07	2.86738E-08	7.16846E-09
100	71	1.1	2968.44	-2897.936	2897.94	2980.247587	1.12589E-07	1.23848E-07	1.36232E-07
101	161	0.085	2859.13	-2698.026	2698.03	2947.416672	1.15111E-07	9.78444E-09	8.31677E-10
102	147	0.13	2863.97	-2716.620	2716.62	2948.872229	1.14997E-07	1.49497E-08	1.94346E-09
D1-1A	1206	2.29	3096.59	-1890.594	1890.59	3018.739005	1.09736E-07	2.51295E-07	5.75466E-07
D1-1B	1641	5.12	3401.37	-1760.372	1760.37	3110.277418	1.03372E-07	5.29263E-07	2.70983E-06
D1-2A	565	1.37	2997.51	-2433.014	2433.01	2988.980934	1.11932E-07	1.53347E-07	2.10085E-07
D1-2B	600	2.29	3096.59	-2496.194	2496.19	3018.739005	1.09736E-07	2.51295E-07	5.75466E-07
D2-1A	3831	3.03	3176.29	654.712	654.71	3042.674844	1.08016E-07	3.27289E-07	9.91686E-07
D2-1B	3162	3.22	3196.75	-34.750	34.75	3048.820533	1.07581E-07	3.46411E-07	1.11544E-06
EC-1A	999	4.49	3333.52	-2334.324	2334.32	3089.89609	1.0474E-07	4.70281E-07	2.11156E-06
EC-1B	1002	4.58	3343.22	-2341.516	2341.52	3092.810725	1.04543E-07	4.78805E-07	2.19293E-06
EC-2A	2030	12.6	4206.93	-2176.934	2176.93	3352.223473	8.89885E-08	1.12126E-06	1.41278E-05
EC-2B	230	5.67	3460.60	-3230.704	3230.70	3128.067569	1.02199E-07	5.7947E-07	3.28559E-06
EC-3A	3810	24.4	5477.74	-1667.740	1667.74	3733.903078	7.17256E-08	1.7501E-06	4.27025E-05
EC-3B	20737	22.1	5230.04	15506.960	15506.96	3659.507901	7.46715E-08	1.65024E-06	3.64703E-05
EC-4A	17065	28.8	5951.60	11113.401	11113.40	3876.224287	6.65552E-08	1.91679E-06	5.52036E-05
EC-4B	3446	7.66	3674.92	-228.918	228.92	3192.435571	9.81196E-08	7.51596E-07	5.75723E-06
LC-1A	728	0.721	2927.62	-2199.420	2199.42	2967.988555	1.13521E-07	8.18485E-08	5.90128E-08
LC-1B	2958	0.964	2953.79	4.210	4.21	2975.848568	1.12922E-07	1.08857E-07	1.04938E-07
MC-1A	2089	9.35	3856.92	-1767.923	1767.92	3247.099853	9.48437E-08	8.86789E-07	8.29148E-06
MC-1B	1409	2.86	3157.98	-1748.980	1748.98	3037.17607	1.08408E-07	3.10046E-07	8.86731E-07
MC-2A	1515	4.98	3386.29	-1871.294	1871.29	3105.749016	1.03673E-07	5.16293E-07	2.57114E-06
MC-2B	2089	14.2	4379.25	-2290.246	2290.25	3403.97664	8.63032E-08	1.22551E-06	1.74022E-05
MC-3A	1358	5.68	3461.68	-2103.681	2103.68	3128.391027	1.02178E-07	5.80372E-07	3.29651E-06
MC-3B	1872	18	4788.49	-2916.489	2916.49	3526.890411	8.03926E-08	1.44707E-06	2.60472E-05
PC-1A	13310	31.1	6199.30	7110.701	7110.70	3950.619464	6.40722E-08	1.99265E-06	6.19713E-05
PC-1B	4611	24.5	5488.51	-877.509	877.51	3737.137651	7.16014E-08	1.75424E-06	4.29788E-05
PC-2A	649	1.24	2983.51	-2334.214	2334.21	2984.775989	1.12247E-07	1.39187E-07	1.72592E-07
PC-2B	207	1.03	2960.90	-2754.197	2754.20	2977.983386	1.1276E-07	1.16143E-07	1.19627E-07
PC-3A	316	1.89	3053.52	-2737.316	2737.32	3005.800713	1.10683E-07	2.0919E-07	3.9537E-07
PC-3B	206	0.604	2915.02	-2708.819	2708.82	2964.204105	1.13811E-07	6.87418E-08	4.152E-08
SUM								4.0319E-06	3.21165E-05
WLS Error Variance								0.004703619	

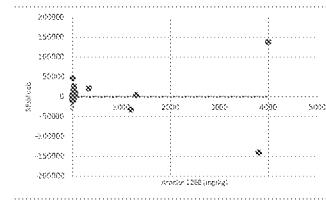
Var =  $\frac{\sum w_i}{((\sum w_i)(\sum w_i x_i^2) - (\sum w_i x_i)^2)}$

WLS Var:OLS Var = 1.09  
Heteroscedasticity not severe

**Case 3a: PCDD/F Concentration and Aroclor 1268 (Original Distribution)**

Location	PCDD/F (ng/kg)	Aroclor 1268 (mg/kg)	Pred PCDD/F (ng/kg)	Pred PCDD/F <sup>2</sup> (ng/kg)	Residual PCDD/F	Residual <sup>2</sup>
36	27038	55	16341.85	267056024.49	10696.05	114305506.42
61	141906	1300	137293.72	18849566843.40	4612.27	21477.0149
68	64192	330	40398.13	185400271.89	21133.87	44664050.85
1718	18409	56	16439.00	2704068717	1970.20	388169.57
BR048	2981	1.4	11134.60	123973945.04	-8153.60	66841249.15
C-15	10834	0.099	11008.21	121189713.19	-174.21	30349.55
C-6	59189	7.58	11734.99	137710015.58	47454.01	225188282.02
131	9396	6.1	11591.21	134356124.40	-2194.84	4817331.09
EPA E3	240329	3800	380168.98	144528451366.00	-139840.78	19555443019.91
EPA F2	94088	1188	126412.91	1598024670.48	32325.21	1044919420.38
EPA H1	538204	4000	399599.00	15967935883.26	138605.20	19211402132.23
GRD MARSH	5980	6.1	11591.21	134356124.40	-561.21	31485666.58
117	2133	11	10627.4	145618387.96	-993.83	58680996.80
110	3049	0.25	11022.88	121503901.93	-7974.28	63589154.86
100	856	1.1	11105.46	12331206.77	10247.97	105057547.71
101	2058	0.085	11006.85	121159770.47	8949.26	80893202.19
102	2678	0.13	11011.22	121247028.08	-833.21	69442315.31
D2-1A	10471	3.03	11292.96	127530903.04	-922.36	676272.87
D2-1B	8782	3.22	11311.42	127948146.32	-2529.32	6397442.65
EC-3A	9344	24.4	13369.06	17731652.37	-4025.36	16239495.13
EC-3B	31228	22.1	13145.61	17280767.59	1982.79	32689727.48
EC-4A	26257	28.8	13796.52	19043859.86	1240.68	155268640.22
EC-4B	9798	7.66	11742.76	137932484.88	-1944.46	3780936.69
LC-1A	6839	0.721	11068.64	125254758.99	-4229.94	17992380.00
LC-1B	15394	0.964	11925.25	123937921.51	4301.55	18593366.74
PC-1A	40766	31.1	14019.96	1965931918	26746.34	71536625.60
PC-1B	18361	24.5	13378.77	17891507.78	4982.03	24920615.08
PC-2A	3534	1.24	11119.06	12633482.75	-7584.66	57527058.77
PC-2B	3473	1.03	11098.66	123180207.52	-7625.36	58464083.33
PC-3A	1691	1.89	11182.21	125041753.44	-9491.21	9093010.36
PC-3B	1128	0.604	11057.27	122263263.46	-9929.70	98598981.25
D1-2A	6945	1.37	11131.69	123934498.87	-4186.79	17529201.71
D1-2B	6285	2.29	11221.07	125912345.57	4935.67	2436809.15

Test for Zero Conditional Mean of Errors



No discernible relationship between residuals and independent variable  
 $\text{Cov}(\hat{y}_i, x_i) = 0$

Tests for Homoscedasticity

BREUSCH-PAGAN SUMMARY OUTPUT

Regression Statistics		$\hat{y}^2 = d_0 + d_1 x$					
Multiple R	0.951750162						
R Square	0.905828371						
Adjusted R Square	0.902790576						
Standard Error	1455898725						
Observations	33						

$H_0$  = homoscedasticity of residuals  
 $H_a$  = heteroscedasticity of residuals  
p<0.05  
Status: Heteroscedastic

ANOVA

	df	SS	MS	F	Significance F
Regression	1	6.32048E+20	6.32048E+20	298.1861914	1.95625E-17
Residual	31	6570894E+19	2.11964E+18		
Total	32	6.97757E+20			

Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%	
Intercept	-159722894.1	268240051.2	-0.595447598	0.555866783	-7068302085.3	387356297.1	-7068302085.3	387356297.1
Aroclor 1268 (mg/kg)	459835.112	26596.2999	17.2806855	1.95625E-17	4044647.888	5128022.337	4044647.888	5128022.337

WHITE'S SUMMARY OUTPUT

Regression Statistics		$\hat{y}^2 = d_0 + \hat{y} \times d_1 + \hat{y}^2 \times d_2$					
Multiple R	0.992866026						
R Square	0.985782946						
Adjusted R Square	0.984825143						
Standard Error	575037466.9						
Observations	33						

$H_0$  = homoscedasticity of residuals  
 $H_a$  = heteroscedasticity of residuals  
p<0.05  
Status: Heteroscedastic

ANOVA

	df	SS	MS	F	Significance F
Regression	2	6.87837E+20	3.43918E+20	104.070938	1.95949E-28
Residual	30	9.52004E+18	3.16668E+17		
Total	32	6.97757E+20			

Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%	
Intercept	388823146.1	137651625.4	2.824689828	0.008333454	107071023	68945269.3	107710123	68945269.3
Pred PCDD/F (ng/kg)	-20202.32708	5300.9799	-3.81505213	0.000640041	-31028.37232	-9376.28134	-31028.37232	-9376.28134
Pred PCDD/F <sup>2</sup>	0.176024473	0.018551756	12.98905303	7.52072E-14	0.148348095	0.20170085	0.148348095	0.20170085

Location	PCDD/F (ng/kg)	Aroclor 1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight	Weight * X	Weight * X <sup>2</sup>
36	27038	55	16341.85	10696.05	8938.760164	1.25154E-08	6.88348E-07	3.78591E-05	
61	141906	1300	137293.72	4612.274	4827.397474	4.30301E-10	5.59392E-07	0.00072299	
68	64192	330	40398.13	21133.87	17852.55555	3.2237E-09	1.06382E-06	0.000951061	
1718	18409	56	16439.00	1970.201	18979.30129	1.24776E-08	6.95942E-07	3.89778E-05	
BR048	2981	1.4	11134.60	-8153.603	8153.60	72481.58591	1.90346E-08	2.66485E-08	3.73079E-09
C-15	10834	0.099	11008.21	-174.211	174.211	72073.23054	1.9252E-08	1.90559E-09	1.86699E-10
C-6	59189	7.58	11734.99	47454.01	47454.01	7443.82402	1.80507E-08	1.36341E-07	1.03713E-06
131	9396	6.1	11591.21	-2194.84	2194.84	7396.40424	1.82727E-08	1.15047E-07	6.8372E-07
EPA E3	240329	3800	380168.98	-139840.78	139840.78	1270630487	6.34155E-11	2.25379E-07	0.000994435
EPA F2	94088	1188	126412.91	32325.213	32325.213	44674.79714	5.01836E-10	5.95239E-09	0.00070744
EPA H1	538204	4000	399599.00	128022.022	128022.022	128022.022	1.26205E-08	2.52027E-09	3.25271E-09
GRD MARSH	5980	6.1	11591.21	-5611.207	5611.21	7396.40164	1.80339E-08	1.11504E-07	6.80172E-07
117	2133	11	10697.24	-9332.931	9332.931	7503.052933	1.75376E-08	1.02255E-07	2.22128E-06
110	3049	0.25	11022.88	7974.281	7974.281	7211.386256	1.92265E-08	1.83665E-09	1.20165E-09
100	856	1.4	11105.46	-849.257	849.257	10240.76	1.09844E-08	2.05932E-08	2.30924E-08
103	2058	0.085	11008.85	-849.257	849.257	7206.630279	1.92544E-08	1.63662E-09	1.29113E-10
102	2678	0.13	11011.22	-833.206	833.206	8333.22	7208.101427	1.94549E-08	2.52020E-09
D2-1A	10471	3.03	11292.96	822.358	822.358	7299.570542	1.87675E-08	5.68654E-08	1.72302E-07
D2-1B	8782	3.22	11211.42	-2519.217	2519.217	7305.563246	1.87367E-08	6.03321E-08	1.04269E-07
EC-3A	9344	24.4	13293.77	-4025.256	4025.256	7873.603296	1.57288E-08	3.82778E-07	9.36419E-06
EC-3B	31228	22.1	13145.61	18082.789	18082.789	18932.79	7091.058326	1.60318E-08	3.54015E-07
EC-4A	26257	28.8	13796.52	12460.684	12460.684	12460.684	81112.38402	1.51951E-08	4.37619E-07
EC-4B	9798	7.66	11742.76	1944.463	1944.463	7445.605715	1.80395E-08	1.38755E-07	1.62604E-06
LC-1A	6839	0.721	11068.64	-4229.339	4229.339	7226.742203	1.91478E-08	1.38054E-08	9.55727E-09
LC-1B	15394	0.964	11029.25	4301.554	4301.554	7234.406693	1.81071E-08	1.84192E-08	1.77561E-08
PC-1A	40766	31.1	14019.96	26746.339	26746.339	1818.228			

**Case 3a: PCDD/F Concentration and Aroclor 1268 (Original Distribution)**

**Iteration #1**

Location	PCDD/F (ng/kg)	Aroclor 1268 (mg/kg)
36	27038	55
61	141908	1300
68	64192	330
1718	18409	56
BR048	2981	1.4
C-15	10834	0.099
C-6	59189	7.58
111	9396	6.1
EPA-E3	240328	3800
EPA-F2	94088	1188
EPA-H1	538204	4000
GRID MARSH	5980	6.1
117	2133	1.1
119	3049	0.25
120	856	1.1
121	2058	0.095
102	2678	0.13
D2-1A	10471	3.03
D2-1B	8782	3.22
EC-3A	9344	24.4
EC-3B	31228	22.1
EC-4A	26257	28.8
EC-4B	7978	7.66
LC-1A	6839	0.721
LC-1B	15394	0.096
PC-1A	40766	31.1
PC-1B	18351	24.5
PC-2A	3534	1.24
PC-2B	3473	1.03
PC-3A	1691	1.89
PC-3B	1128	0.604
DI-2A	6945	1.37
DI-2B	6285	2.29

Weighted Least Squares performed with "Real Stats" Add-In

$$Pred Y_i' = Abs(Res)x + \delta_1$$

$$W_i = \frac{1}{Pred Y_i'^2}$$

WLS solution is asymptotic at iteration #4.

**Iteration #2**

Location	PCDD/F (ng/kg)	Aroclor 1268 (mg/kg)	Pred Y	Residual	Abs(Res)	Pred Y'	Weight
36	27038	55	1.63E+04	1.07E+04	8.94E+03	1.25154E-08	
61	141908	1300	1.37E+05	4.61E+04	4.82E+04	4.02E+02	
68	64192	330	4.23E+04	2.35E+04	1.78E+04	3.23271E-09	
1718	18409	56	1.64E+04	1.97E+03	8.97E+03	1.24277E-08	
BR048	2981	1.4	1.11E+04	8.215E+03	8.15E+03	1.90248E-08	
C-15	10834	0.099	1.10E+04	1.74E+02	1.74E+02	1.30252E-08	
C-6	59189	7.58	1.77E+04	4.75E+04	7.44E+03	1.80507E-08	
111	9396	6.1	1.16E+04	-2.19E+03	7.40E+03	1.82793E-08	
EPA-E3	240328	3800	3.80E+05	-1.40E+05	1.40E+05	6.19151E-11	
EPA-F2	94088	1188	1.26E+05	3.23E+04	4.47E+04	5.01043E-10	
EPA-H1	538204	4000	4.00E+05	1.39E+05	1.33E+05	5.62025E-11	
GRID MARSH	5980	6.1	1.16E+04	-5.61E+03	5.61E+03	1.82793E-08	
117	2133	1.1	1.23E+04	-9.93E+03	9.93E+03	7.55E+03	1.75873E-08
119	3049	0.25	1.10E+04	-7.97E+03	7.97E+03	7.21E+02	1.92266E-08
120	856	1.1	1.00E+04	-7.00E+03	7.00E+03	6.90E+02	1.84150E-08
121	2058	0.095	1.05E+04	-8.95E+03	8.95E+03	7.21E+02	1.92544E-08
122	2678	0.13	1.08E+04	-8.30E+03	8.30E+03	7.21E+02	1.92488E-08
D2-1A	10471	3.03	1.23E+04	-8.22E+02	8.22E+02	7.30E+03	1.87675E-08
D2-1B	8782	3.22	1.13E+04	-2.55E+03	7.31E+03	1.78367E-08	
EC-3A	9344	24.4	1.34E+04	4.03E+03	7.97E+03	1.57296E-08	
EC-3B	31228	22.1	1.31E+04	1.81E+04	7.90E+03	1.60188E-08	
EC-4A	26257	28.8	1.38E+04	1.25E+04	8.13E+03	1.51951E-08	
EC-4B	7978	7.66	1.77E+04	-5.94E+03	5.94E+03	7.45E+03	1.80385E-08
LC-1A	6839	0.721	1.11E+04	-4.23E+03	4.23E+03	7.23E+02	1.91476E-08
LC-1B	15394	0.964	1.13E+04	4.50E+03	7.23E+03	1.91071E-08	
PC-1A	40766	31.1	1.40E+04	2.67E+04	7.67E+04	8.18969E-08	
PC-1B	18351	24.5	1.24E+04	4.49E+03	7.69E+03	1.90299E-08	
PC-2A	3534	1.24	1.15E+04	-7.58E+03	7.58E+03	7.24E+02	1.90512E-08
PC-2B	3473	1.03	1.15E+04	-7.63E+03	7.63E+03	7.24E+02	1.90867E-08
PC-3A	1691	1.89	1.22E+04	-9.49E+03	9.49E+03	7.28E+02	1.89537E-08
PC-3B	1128	0.604	1.21E+04	-9.93E+03	9.93E+03	7.22E+02	1.91672E-08
DI-2A	6945	1.37	1.21E+04	-4.19E+03	4.19E+03	7.25E+03	1.90396E-08
DI-2B	6285	2.29	1.12E+04	-4.94E+03	4.94E+03	7.28E+03	1.89881E-08

**OVERALL FIT**

Multiple R	0.58417537	AIC	32.08906335
R Square	0.34156508	AICc	32.46906335
Adjusted R Square	0.32067527	BSC	33.56570931
Standard Error	1.62715855	Observations	33

**ANOVA**

	df	ss	MS	F	p-value	sig
Regression	1	42.5215429	42.52154	16.05960	0.00039	yes
Residual	31	82.07974702	2.64773			
Total	32	124.6012913				

**coeff**

Intercept	std err	t stat	p value	lower	upper	vif
10585.7005	2328.574909	4.55E+00	7.78E-05	5.84E+03	1.53E+04	1

**Aroclor 1268 (mg/kg)**

Intercept	std err	t stat	p value	lower	upper	vif
108.4637	27.0655148	4.01E+00	3.54E-04	5.33E+01	1.64E+02	1

**Iteration #3**

Location	PCDD/F (ng/kg)	Aroclor 1268 (mg/kg)	Pred Y	Residual	Abs(Res)	Pred Y'	Weight
36	27038	55	1.63E+04	1.07E+04	8.94E+03	1.25154E-08	
61	141908	1300	1.37E+05	4.61E+04	4.82E+04	4.02E+02	
68	64192	330	4.23E+04	1.79E+03	1.78E+03	1.92371E-09	
1718	18409	56	1.64E+04	1.97E+03	8.97E+03	1.24277E-08	
BR048	2981	1.4	1.11E+04	8.215E+03	8.15E+03	1.90248E-08	
C-15	10834	0.099	1.10E+04	1.74E+02	1.74E+02	1.30252E-08	
C-6	59189	7.58	1.77E+04	4.75E+04	7.44E+03	1.80507E-08	
111	9396	6.1	1.16E+04	-2.19E+03	7.40E+03	1.82793E-08	
EPA-E3	240328	3800	3.23E+05	3.23E+04	4.47E+04	5.01043E-10	
EPA-F2	94088	1188	1.26E+05	3.23E+04	4.47E+04	5.04E+04	
EPA-H1	538204	4000	4.43E+05	9.55E+04	9.55E+04	5.59819E-11	
GRID MARSH	5980	6.1	1.13E+04	7.96E+03	7.96E+03	1.74266E-08	
117	2133	1.1	1.38E+04	-9.66E+03	9.66E+03	7.72E+02	1.67698E-08
119	3049	0.25	1.07E+04	-7.00E+03	7.00E+03	6.90E+02	1.84150E-08
120	856	1.1	1.67E+04	-9.87E+03	9.87E+03	1.82451E-08	
121	2058	0.095	1.08E+04	-8.95E+03	8.95E+03	1.92544E-08	
122	2678	0.13	1.08E+04	-8.56E+03	8.56E+03	1.90401E-08	
D2-1A	10471	3.03	1.23E+04	-7.04E+03	7.04E+03	1.83970E-08	
D2-1B	8782	3.22	1.10E+04	-2.17E+03	7.27E+03	7.47E+03	
EC-3A	9344	24.4	1.32E+04	-3.90E+03	8.14E+03	1.50961E-08	
EC-3B	31228	22.1	1.30E+04	-1.82E+04	8.07E+03	1.53691E-08	
EC-4A	26257	28.8	1.37E+04	1.25E+04	8.28E+03	1.45937E-08	
EC-4B	7978	7.66	1.34E+04	-1.63E+03	6.71E+03	1.72656E-08	
LC-1A	6839	0.721	1.07E+04	-3.84E+03	3.84E+03	1.83042E-08	
LC-1B	15394	0.964	1.13E+04	4.50E+03	7.61E+03	1.83042E-08	
PC-1A	40766	31.1	1.40E+04	2.67E+04	7.67E+04	8.18969E-08	
PC-1B	18351	24.5	1.24E+04	4.49E+03	7.69E+03	1.90512E-08	
PC-2A	3534	1.24	1.15E+04	-5.11E+03	5.11E+03	1.50844E-08	
PC-2B	3473	1.03	1.07E+04	-8.14E+03	8.14E+03	1.84053E-08	
PC-3A	1691	1.89	1.22E+04	-9.12E+03	7.43E+03	1.81222E-08	
PC-3B	1128	0.604	1.21E+04	-9.54E+03	7.93E+03	1.83222E-08	
DI-2A	6945	1.37	1.09E+04	-3.81E+03	3.81E+03	7.44E+03	1.82031E-08
DI-2B	6285	2.29	1.09E+04	4.57E+03	4.57E+03	7.44E+03	1.819E-08

**OVERALL FIT**

Multiple R	0.58901378	AIC	30.7295874
R Square	0.346953723	AICc	31.12958745
Adjusted R Square	0.32652902	BSC	32.20946631
Standard Error	1.595495124	Observations	33

**ANOVA**

	df	ss	MS	F	p-value	sig
Regression	1	41.8499789	41.84900	16.46864	0.00031	yes
Residual	31	78.77512074	2.54113			
Total	32	120.6241186				

**coeff**

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**Case 3a: PCDD/F Concentration and Aroclor 1268 (Original Distribution)**

Location	PCDD/F (ng/kg)	Aroclor 1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight	Weight * X	Weight*X^2
36	27038	55	16547.83	10490.071	10490.07	9105.730375	1.20606E-08	6.63335E-07	3.64834E-05
61	141906	1300	151080.61	-9174.616	9174.62	48412.39425	4.26665E-10	5.54664E-07	0.000721064
68	64192	330	46263.91	17928.093	17928.09	17787.92521	3.16045E-09	1.04295E-06	0.000344173
1718	18409	56	16655.89	1753.313	1753.31	9137.301993	1.19774E-08	6.70737E-07	3.75613E-05
BR048	2981	1.4	10755.90	-7774.895	7774.90	7413.491674	1.81951E-08	2.54731E-08	3.56624E-08
C-15	10834	0.099	10615.31	218.689	218.69	7372.416999	1.83984E-08	1.82144E-09	1.80323E-10
C-6	59189	7.58	11423.70	47765.303	47765.30	7608.60427	1.72739E-08	1.30936E-07	9.92495E-07
111	9396	6.1	11263.77	-1867.403	1867.40	7561.878276	1.7488E-08	1.06677E-07	6.50729E-07
EPA-E3	240328	3800	421226.77	-180898.570	180898.57	127341.4382	6.16681E-11	2.34339E-07	0.000890487
EPA-F2	94088	1188	138978.07	-44890.367	44890.37	44876.37308	4.96552E-10	5.89903E-07	0.000700805
EPA-H1	538204	4000	442838.46	95365.738	95365.74	133655.7617	5.59789E-11	2.23916E-07	0.000895663
GRID MARSH	5980	6.1	11263.77	-5283.770	5283.77	7561.878276	1.7488E-08	1.06677E-07	6.50729E-07
117	2133	11	11793.26	-9659.843	9659.84	7716.579202	1.67939E-08	1.84732E-07	2.03206E-06
110	3049	0.25	10631.63	-7583.028	7583.03	7377.184313	1.83746E-08	4.59366E-09	1.14841E-09
100	856	1.1	10723.48	-9867.778	9867.78	7404.020188	1.82417E-08	2.00658E-08	2.20724E-08
101	2058	0.085	10613.80	-8556.204	8556.20	7371.974997	1.84006E-08	1.56405E-09	1.32944E-10
102	2678	0.13	10618.66	-7940.644	7940.64	7373.395719	1.83935E-08	2.39116E-09	3.10851E-10
D2-1A	10471	3.03	10932.03	-461.431	461.43	7464.95341	1.79451E-08	5.43736E-08	1.64752E-07
D2-1B	8782	3.22	10952.56	-2170.462	2170.46	7470.952018	1.79163E-08	5.76905E-08	1.85763E-07
EC-3A	9344	24.4	13241.24	-3897.540	3897.54	8139.638878	1.50935E-08	3.68281E-07	8.98606E-06
EC-3B	31228	22.1	12992.71	18235.694	18235.69	8067.024157	1.53664E-08	3.39598E-07	7.50512E-06
EC-4A	26257	28.8	13716.70	12540.503	12540.50	8278.553995	1.45912E-08	4.20227E-07	1.21025E-05
EC-4B	9798	7.66	11432.34	-1634.041	1634.04	7611.13	1.72624E-08	1.3223E-07	1.01288E-06
LC-1A	6839	0.721	10682.52	-3843.824	3843.82	7392.054545	1.83008E-08	1.31949E-08	9.5135E-09
LC-1B	15394	0.964	10708.78	4685.018	4685.02	7399.726448	1.82629E-08	1.76054E-08	1.69716E-08
PC-1A	40766	31.1	13965.23	26801.068	26801.07	8351.168715	1.43386E-08	4.45929E-07	1.38684E-05
PC-1B	18361	24.5	13252.05	5108.754	5108.75	8142.796039	1.50818E-08	3.69504E-07	9.05284E-06
PC-2A	3534	1.24	10738.61	-7204.206	7204.21	7408.440215	1.82199E-08	2.25927E-08	2.80149E-08
PC-2B	3473	1.03	10715.91	-7242.614	7242.61	7401.810175	1.82526E-08	1.88002E-08	1.93642E-08
PC-3A	1691	1.89	10808.84	-9117.844	9117.84	7428.961766	1.81194E-08	3.42457E-08	6.47243E-08
PC-3B	1128	0.604	10669.88	-9542.311	9542.31	7388.360666	1.83191E-08	1.10647E-08	6.6831E-09
D1-2A	6945	1.37	10752.65	-3807.754	3807.75	7412.544525	1.81997E-08	2.49337E-08	3.41591E-08
D1-2B	6285	2.29	10852.07	-4566.667	4566.67	7441.590413	1.8058E-08	4.13527E-08	9.46977E-08

SUM      4.80615E-07      6.9364E-06      0.003683775

WLS Error Variance      279  

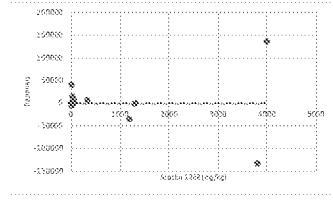
$$Var = \frac{\sum w_i}{((\sum w_i)(\sum w_i x_i^2) - (\sum w_i x_i)^2)}$$

WLS Var:OLS Var =	1.01
Heteroscedasticity not severe	

**Case 3b: Furan Congener Concentration and Aroclor 1268 (Original Distribution)**

Location	Furan (ng/kg)	Aroclor 1268 (mg/kg)	Pred PCDD/F (ng/kg)	Pred PCDF/P2 (ng/kg)	Residual PCDD/F	Residual PCDF/P2
36	14468	55	8709.95	7583267.95	5758.05	33155113.15
61	122400	1300	123061.00	15144010951.22	-661.01	436928.62
68	40850	330	33968.22	1153839753.42	6881.78	4735926.89
1718	8750	56	9801.80	77471691.53	51.80	2653.28
BRO48	391	1.4	3786.89	14340512.01	-3395.89	11532047.48
C-15	1348	0.099	3667.29	13497662.25	-2319.29	5379580.60
C-6	44710	7.58	4354.51	18961748.11	40355.49	1628565624.75
111	5936	6.1	4218.57	17796362.82	817.51	66818.43
EPA-E3	219200	3800	352681.91	12438430590.77	-13348.17	1781735310.17
EPA-F2	77700	1188	112774.00	12717975592.91	-35074.00	123015636.76
EPA-H1	597600	4000	371051.24	137679021679.71	136548.76	1864556425.05
GRID MARSH	3690	6.1	4218.57	17796362.82	528.57	27939.08
117	148	11	4668.63	21796105.18	-4521.02	2043939.05
110	630	0.25	3681.26	13551685.34	-3051.26	931019.00
100	71	1.1	3759.33	14132579.93	-3688.83	13697484.32
101	161	0.095	3666.11	13440336.29	-3505.01	1285577.02
102	147	0.13	3670.24	13470658.66	-3522.89	12410376.98
D2-1A	3831	3.03	3936.60	15496815.40	-105.60	1151.25
D2-1B	3162	3.22	3954.05	15634516.44	-792.05	67344.21
EC-3A	3810	24.4	5899.40	43802876.12	-2089.40	4365576.69
EC-3B	20737	22.1	5688.15	32359497.07	15048.85	2284680274.8
EC-4A	17065	28.3	6303.53	9734471.34	10761.47	115309269.20
EC-4B	3446	7.66	4361.86	19025794.74	-915.86	838793.68
LC-3A	728	0.721	3724.52	13872063.37	-2996.32	8977944.92
LC-3B	2958	0.964	3746.84	1403811.62	-788.84	622270.15
PC-1A	13310	31.1	6514.78	42442350.94	6795.22	46175922.68
PC-1B	4611	24.5	5908.58	34911330.30	-1975.85	1683716.64
PC-2A	649	1.24	3772.19	1429425.93	-3122.89	9752449.02
PC-2B	207	1.03	3752.90	14098280.95	-3546.20	12575555.73
PC-3A	316	1.89	3831.89	14683400.01	-3515.69	12360939.64
PC-3B	206	0.604	3713.78	13792129.61	-3507.58	12393986.97
D1-2A	565	1.37	3784.13	14319650.47	-3219.63	10366026.37
D1-2B	600	2.29	3868.63	14966311.84	-3268.23	10681338.96

Test for Zero Conditional Mean of Errors



No discernible relationship between residuals and independent variable  
 $\text{Cov}(0, x) = 0$

Tests for Homoscedasticity

BREUSCH-PAGAN SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.955872222
R Square	0.913691705
Adjusted R Square	0.910937566
Standard Error	1314852.258
Observations	33

$$\hat{y}^2 = d_0 + x_1 d_1$$

$H_0$  = homoscedasticity of residuals  
 $H_a$  = heteroscedasticity of residuals  
p<0.05  
Status: Heteroscedastic

ANOVA

	df	ss	ms	f	Significance F
Regression	1	5.679351E+20	5.673651E+20	329.1775262	4.78561E-18
Residual	31	5.35938E+19	1.72884E+18		
Total	32	6.20955E+20			

Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%
Intercept	-22652.90474	24225319.4	-0.093546357	0.356239866	7207.7620
Aroclor 1268 (mg/kg)	4345324.053	239805.5129	18.15167074	4.78561E-18	3856135.714

$H_0$  = homoscedasticity of residuals  
 $H_a$  = heteroscedasticity of residuals  
p<0.05  
Status: Heteroscedastic

WHITE'S SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.996252922
R Square	0.992519884
Adjusted R Square	0.992021209
Standard Error	393482191.6
Observations	33

$$\hat{y}^2 = d_0 + \hat{Y} \times d_1 + \hat{Y}^2 \times d_2$$

$H_0$  = homoscedasticity of residuals  
 $H_a$  = heteroscedasticity of residuals  
p<0.05  
Status: Heteroscedastic

ANOVA

	df	ss	ms	f	Significance F
Regression	2	6.36314E+20	3.08157E+20	1990.31645	3.28418E-32
Residual	30	4.64485E+18	1.54828E+17		
Total	32	6.20955E+20			

Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%
Intercept	158689740.7	79912486.65	1.985794953	0.056261391	4513229.628
Pred PCDD/F (ng/kg)	-1692.14828	3699.388975	-4.592610312	7.34139E-05	24548.32964
Pred PCDF/P2	1.034465108	17.78063223	1.76199E-17	0.163279445	0.205053772

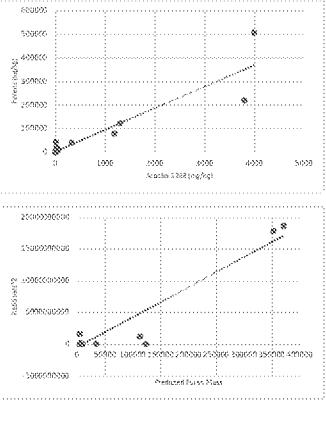
$H_0$  = homoscedasticity of residuals  
 $H_a$  = heteroscedasticity of residuals  
p<0.05  
Status: Heteroscedastic

OLS Error Variance

Location	Furan (ng/kg)	Aroclor 1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight	Weight * X	Weight * Y
36	14468	55	8709.95	5758.05	5758.05	4770.515655	4.394391E-08	2.41656E-08	0.00132321
61	122400	1300	123061.00	-464.06	464.06	4425313175	5.11168E-09	0.51510E-07	0.00395874
68	40850	330	33968.22	6881.78	6881.78	1348649451	5.49759E-08	1.81438E-06	0.003958728
1718	8750	56	9801.80	51.80	51.80	4802.210305	4.33679E-08	2.42476E-06	0.00135956
BRO48	391	1.4	3786.89	-3395.83	3395.83	3935.89	3.07933E-03	1.02889E-07	1.48373E-07
C-15	1348	0.099	3667.29	2319.39	2319.39	3039.457516	1.07881E-07	3.778E-07	2.07731E-07
C-6	44710	7.58	4354.51	5285.74	5285.74	3210.650326	9.64076E-09	5.88086E-07	3.59723E-06
111	5936	6.1	4218.57	4521.02	4521.02	3375.958941	8.77168E-08	9.65158E-07	1.06167E-05
110	630	0.25	3681.26	3051.26	3051.26	3052.42381	1.05467E-07	2.71364E-08	6.78411E-09
100	71	1.1	3759.33	3688.32	3688.32	3062.133681	1.06644E-07	1.17209E-07	1.29045E-07
101	161	0.095	3666.11	3505.07	3505.07	3509.013793	1.08921E-07	9.25827E-09	7.86953E-10
102	147	0.13	3670.24	3522.88	3522.88	3021.440044	1.08818E-07	1.41464E-08	1.83930E-09
D2-1A	3831	3.03	3935.60	-105.59	105.60	3123.25401	1.05098E-07	3.10599E-07	9.41115E-07
D2-1B	3162	3.23	3954.05	-793.051	793.051	3139.275959	1.02148E-07	2.28986E-07	1.05978E-06
EC-3A	2958	24.4	5995.40	5995.40	5995.40	2093.949	3.00334297	6.31125E-08	1.05978E-06
EC-3B	20737	22.1	5688.15	15048.855	15048.855	3777.767567	7.3619E-08	1.59036E-06	3.15469E-06
EC-4A	17065	28.8	6303.53	10761.472	10761.472	3940.120521	6.44141E-08	1.85513E-06	5.34276E-05
EC-4B	3446	7.66	4361.86	-915.85	915.85	3270.099409	9.35143E-08	7.16321E-07	5.48701E-06
LC-3A	728	0.721	3724.52	-2996.322	2996.322	3059.17477	1.07486E-07	7.74973E-08	5.58756E-08
LC-3B	2958	0.964	3746.84	-788.841	788.841	3057.373233	1.06945E-07	1.03095E-07	9.33337E-08
PC-1A	13310	31.1	6514.78	6795.22	6795.22	4013.017804	6.20952E-08	1.93116E-06	6.00591E-05
PC-1B	4611	24.5	5908.58	-1297.581	1297.581	3803.334297	6.31125E-08	1.69326E-06	4.14948E-05
PC-2A	649	1.24	3772.19	-312.891	312.891	3066.629997	1.06336E-07	1.33856E-07	1.63592E-07
PC-2B	207	1.03	3752.90	-546.203	546.203	3059.953063	1.06799E-07	1.10003E-07	1.13303E-07
PC-3A	316	1.89	3831.89	-3515.692	3515.692	3087.223113	1.04921E-07	1.98301E-07	3.74795E-07
PC-3B	206	0.604	3713.78	-3507.576	3507.576	3046.463223	1.07748E-07	6.50796E-08	3.93081E-08
D1-2A	565	1.37	3784.13	-3219.631	3219.631	3070.741188	1.06051E-07	1.45289E-07	1.99047E-07
D1-2B	600	2.29	3868.63	-3268.232	3268.232	3099.900101	1.04065E-07	2.33309E-07	5.45272E-07

SUM 2.60139E-06 2.2891E-05 0.00475124

$$Var = \frac{\sum w_i}{(\sum w_i)(\sum w_i^2) - (\sum w_i)^2}$$



**Case 3a: PCDD/F Concentration and Aroclor 1268 (Original Distribution)**

**Iteration #1**      **Iterations (n)**      **Aroclor 1268 (mg/kg)**

Location	Furnace (mg/kg)	Aroclor 1268 (mg/kg)
36	14468	55
61	122400	1300
68	40850	330
1718	8750	56
BRO48	391	1.4
C-15	1348	0.099
C-6	44710	7.58
111	5036	6.1
EPA-E3	219200	3800
EPA-F2	77700	1188
EPA-H1	507600	4000
GRID MARSH	3690	6.1
117	148	0.11
119	630	0.25
120	74	1.1
121	161	0.095
102	147	0.13
D2-1A	3831	3.03
D2-1B	3162	3.22
EC-3A	3810	24.4
EC-3B	20737	22.1
EC-4A	17065	28.8
EC-4B	3446	7.66
LC-1A	728	0.721
LC-1B	2958	0.98
PC-1A	33110	31.1
PC-1B	46511	24.5
PC-2A	649	1.24
PC-2B	207	1.03
PC-3A	316	1.89
PC-3B	206	0.604
DI-2A	565	1.37
DI-2B	600	2.29

Weighted Least Squares performed with "Real Stats" Add-In

$$Pred Y_i' = Abs(Res)x + \theta_1$$

$$W_i = \frac{1}{Pred Y_i'^2}$$

WLS solution is asymptotic at iteration #4.

**Iteration #2**

Location	Furnace (mg/kg)	Aroclor 1268 (mg/kg)	Pred Y	Residual	Abs(Res)	Pred Y'	Weight
36	14468	55	8.71E+03	5.76E+03	4.77E+03	4.39409E-08	
61	122400	1300	1.40E+05	6.68E+02	4.42E+04	5.01164E+02	
68	40850	330	3.40E+04	5.88E+03	1.31E+04	3.09936E-08	
1718	8750	56	8.89E+03	5.19E+03	4.80E+03	4.59326E-08	
BRO48	391	1.4	3.79E+03	3.40E+03	3.40E+03	1.05982E-07	
C-15	1348	0.099	3.67E+03	-2.32E+03	3.22E+03	3.03E+03	1.08898E-07
C-6	44710	7.58	4.35E+03	4.94E+04	3.27E+03	3.63595E-08	
111	5036	6.1	4.22E+03	8.28E+02	3.22E+03	9.64706E-08	
EPA-E3	219200	3800	5.53E+05	-1.33E+05	1.23E+05	6.55999E-11	
EPA-F2	77700	1188	1.13E+05	3.51E+04	4.07E+04	6.04269E-10	
EPA-H1	507600	4000	3.71E+05	1.37E+05	1.30E+05	5.93493E-11	
GRID MARSH	3690	6.1	4.22E+03	-5.29E+02	3.22E+03	9.64706E-08	
117	148	0.11	4.67E+03	4.52E+03	3.53E+03	8.77416E-08	
119	630	0.25	5.68E+03	-5.05E+03	3.04E+03	1.08546E-07	
120	74	1.1	5.70E+03	5.85E+03	3.00E+03	1.08546E-07	
121	161	0.095	5.67E+03	5.21E+03	3.03E+03	1.08932E-07	
122	147	0.13	5.67E+03	-3.62E+03	3.03E+03	1.08932E-07	
D2-1A	3831	3.03	3.84E+03	-1.06E+02	3.12E+03	1.02509E-07	
D2-1B	3162	3.22	3.95E+03	-7.92E+02	3.13E+03	1.02114E-07	
EC-3A	3810	24.4	5.90E+03	2.09E+03	2.08E+03	6.92795E-08	
EC-3B	20737	22.1	5.69E+03	1.50E+04	3.73E+03	7.19619E-08	
EC-4A	17065	28.8	6.30E+03	1.19E+04	3.98E+03	6.44141E-08	
EC-4B	3446	7.66	4.36E+03	9.16E+02	9.16E+02	3.95143E-08	
LC-1A	728	0.721	3.72E+03	-3.60E+03	3.00E+03	1.07486E-07	
LC-1B	2958	0.98	3.75E+03	7.89E+02	3.06E+03	1.06945E-07	
PC-1A	33110	31.1	6.51E+03	6.80E+03	3.60E+03	6.20952E-08	
PC-1B	46511	24.5	5.93E+03	1.35E+04	3.80E+03	6.03488E-08	
PC-2A	649	1.24	3.77E+03	-2.32E+03	3.12E+03	1.00346E-07	
PC-2B	207	1.03	3.75E+03	-3.65E+03	3.06E+03	1.05799E-07	
PC-3A	316	1.89	3.81E+03	-3.52E+03	3.09E+03	1.04921E-07	
PC-3B	206	0.604	3.73E+03	-3.51E+03	3.50E+03	1.07474E-07	
DI-2A	565	1.37	3.72E+03	-3.22E+03	3.22E+03	1.08051E-07	
DI-2B	600	2.29	3.87E+03	-3.27E+03	3.27E+03	1.04065E-07	

**OVERALL FIT**

Multiple R	0.44961362	AIC	61.52760290
R Square	0.20215241	AICc	61.52760290
Adjusted R Square	0.17771967	BSC	63.02411046
Standard Error	2.52461621		
Observations	33		

**ANOVA**

	df	ss	MS	F	p-value	tstat	df	ss	MS	F	p-value	tstat
Regression	1	50,77878362	50,778783	7,85454	0.020866	yes	1	42,3635592	42,363558	10,05335102	0.0034215	yes
Residual	31	200,4181133	6,46490				31	130,6301055	4,213874			
Total	32	251,1905969					32	172,9953687				

**coeff**

Intercept	std err	tstat	p-value	lower	upper	vif
3849.9211	1611.016205	2.39E+00	2.02E+02	8.56E+02	2.89E+01	1.83E+02

**Aroclor 1268 (mg/kg)**

Intercept	std err	tstat	p-value	lower	upper	vif
105.7150	37,72040404	2.80E+00	8.56E-03	2.89E+01	1.83E+02	1

**Iteration #3**

Location	Furnace (mg/kg)	Aroclor 1268 (mg/kg)	Pred Y	Residual	Abs(Res)	Pred Y'	Weight
36	14468	55	8.71E+03	5.76E+03	4.77E+03	4.39409E-08	
61	122400	1300	1.35E+05	-1.25E+04	4.51E+04	4.91725E+10	
68	40850	330	3.72E+03	3.69E+03	1.20E+03	4.67983E-09	
1718	8750	56	9.62E+03	8.71E+02	5.64E+03	3.38293E-08	
BRO48	391	1.4	4.13E+03	3.74E+03	3.70E+03	7.31907E-08	
C-15	1348	0.099	4.00E+03	2.65E+03	3.65E+03	7.49808E-08	
C-6	44710	7.58	4.75E+03	4.00E+04	4.80E+03	3.65703E-08	
111	5036	6.1	4.80E+03	4.21E+02	4.21E+02	3.85898E-08	
EPA-E3	219200	3800	3.86E+05	-1.67E+05	1.25E+05	4.62926E-11	
EPA-F2	77700	1188	1.23E+05	4.57E+03	4.57E+03	5.79592E+10	
EPA-H1	507600	4000	4.06E+05	1.02E+05	1.31E+05	5.81877E+11	
GRID MARSH	3690	6.1	4.69E+03	1.51E+02	4.15E+03	3.855E+08	
117	148	0.11	5.10E+03	4.95E+03	4.00E+03	6.24256E-08	
119	630	0.25	5.08E+03	4.30E+03	3.60E+03	6.24256E-08	
120	74	1.1	4.65E+03	4.03E+03	3.69E+03	7.35705E-08	
121	161	0.095	3.84E+03	3.64E+03	3.65E+03	4.78791E-08	
122	147	0.13	3.86E+03	3.86E+03	3.68E+03	7.48204E-08	
D2-1A	3831	3.03	4.30E+03	-4.65E+02	4.65E+03	3.75705E-08	
D2-1B	3162	3.22	4.32E+03	-1.53E+03	3.75E+03	7.09455E-08	
EC-3A	3810	24.4	6.44E+03	-2.63E+03	4.43E+03	5.09658E-08	
EC-3B	20737	22.1	6.21E+03	1.45E+04	4.36E+03	5.26951E-08	
EC-4A	17065	28.8	6.89E+03	1.02E+04	4.57E+03	4.78943E-08	
LC-1A	728	0.721	4.76E+03	1.32E+03	3.90E+03	6.58939E-08	
LC-1B	2958	0.98	4.80E+03	1.17E+03	3.90E+03	6.42486E-08	
PC-1A	33110	31.1	7.52E+03	-6.35E+02	4.65E+03	4.63948E-08	
PC-1B	46511	24.5	6.45E+03	1.84E+03	4.43E+03	5.09917E-08	
PC-2A	649	1.24	4.21E+03	-3.67E+03	3.69E+03	7.33927E-08	
PC-2B	207	1.03	4.20E+03	-3.69E+03	3.68E+03	7.35923E-08	
PC-3A	316	1.89	4.18E+03	-3.87E+03	3.71E+03	7.25598E-08	
PC-3B	206	0.604	4.05E+03	-3.85E+03	3.67E+03	7.20258E-08	
DI-2A	565	1.37	4.13E+03	-3.58E+03	3.58E+03	7.32282E-08	
DI-2B	600	2.29	4.22E+03	-3.62E+03	3.62E+03	7.20795E-08	

**OVERALL FIT**

Multiple R	0.48542350	AIC	50,37002219
R Square	0.23565397	AICc	50,37002219
Adjusted R Square	0.21174960	BSC	51,86629724
Standard Error	2.14714554		
Observations	33		

**ANOVA**

	df	ss	MS	F	p-value	tstat	df	ss	MS	F	p-value	tstat
Regression	1	44,05812539	44,05813	9,55659	0.00419	yes	1	4,38E+01	4,375515	9,64043159	0.004046	

**Case 3a: PCDD/F Concentration and Aroclor 1268 (Original Distribution)**

Location	Furans (ng/kg)	Aroclor 1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight	Weight * X	Weight*X^2
36	14468	55	9539.70	4928.297	4928.30	5432.161848	3.38887E-08	1.86388E-06	0.000102513
61	122400	1300	135616.91	-13216.910	13216.91	45150.49863	4.90541E-10	6.37703E-07	0.000829013
68	40850	330	37388.08	3461.917	3461.92	14205.28845	4.95564E-09	1.63536E-06	0.000539669
1718	8750	56	9640.97	-890.970	890.97	5464.064127	3.34941E-08	1.87567E-06	0.000105038
BR048	391	1.4	4111.80	-3720.801	3720.80	3722.199719	7.21773E-08	1.01048E-07	1.41468E-07
C-15	1348	0.099	3980.05	-2632.053	2632.05	3680.694854	7.38143E-08	7.30761E-09	7.23454E-10
C-6	44710	7.58	4737.63	39972.370	39972.37	3919.3558	6.50984E-08	4.93446E-07	3.74032E-06
111	5036	6.1	4587.76	448.326	448.33	3872.140428	6.66957E-08	4.06844E-07	2.48175E-06
EPA-E3	219200	3800	388783.99	-169583.988	169583.99	124906.195	6.40962E-11	2.43565E-07	0.000925549
EPA-F2	77700	1188	124275.02	-46575.024	46575.02	41577.44344	5.78475E-10	6.87228E-07	0.000816427
EPA-H1	507600	4000	409037.35	98562.645	98562.65	131286.6507	5.80175E-11	2.3207E-07	0.00092828
GRID MARSH	3690	6.1	4587.76	-897.755	897.76	3872.140428	6.66957E-08	4.06844E-07	2.48175E-06
117	148	11	5083.96	-4936.355	4936.35	4028.461593	6.162E-08	6.7782E-07	7.45602E-06
110	630	0.25	3995.34	-3365.344	3365.34	3685.512098	7.36214E-08	1.84054E-08	4.60134E-09
100	71	1.1	4081.42	-4010.921	4010.92	3712.629035	7.25499E-08	7.98049E-08	8.77854E-08
101	161	0.085	3978.64	-3817.536	3817.54	3680.248222	7.38322E-08	6.27574E-09	5.33438E-10
102	147	0.13	3983.19	-3835.840	3835.84	3681.683825	7.37746E-08	9.5907E-09	1.24679E-09
D2-1A	3831	3.03	4276.87	-445.866	445.87	3774.200433	7.02021E-08	2.12712E-07	6.44518E-07
D2-1B	3162	3.22	4296.11	-1134.107	1134.11	3780.261866	6.99771E-08	2.25326E-07	7.25551E-07
EC-3A	3810	24.4	6440.94	-2630.938	2630.94	4455.952125	5.03639E-08	1.22888E-06	2.99846E-05
EC-3B	20737	22.1	6208.02	14528.976	14528.98	4382.576884	5.20644E-08	1.15062E-06	2.54288E-05
EC-4A	17065	28.8	6886.51	10178.488	10178.49	4596.322151	4.73346E-08	1.36324E-06	3.92612E-05
EC-4B	3446	7.66	4745.73	-1299.731	1299.73	3921.907982	6.50137E-08	4.98005E-07	3.81472E-06
LC-1A	728	0.721	4043.04	-3314.841	3314.84	3700.538071	7.30248E-08	5.26509E-08	3.79613E-08
LC-1B	2958	0.964	4067.65	-1109.649	1109.65	3708.290325	7.27198E-08	7.01019E-08	6.75782E-08
PC-1A	13310	31.1	7119.43	6190.574	6190.57	4669.697391	4.58588E-08	1.42621E-06	4.43551E-05
PC-1B	4611	24.5	6451.06	-1840.065	1840.06	4459.142353	5.02918E-08	1.23215E-06	3.01877E-05
PC-2A	649	1.24	4095.60	-3446.298	3446.30	3717.095354	7.23757E-08	8.97458E-08	1.11285E-07
PC-2B	207	1.03	4074.33	-3867.632	3867.63	3710.395875	7.26373E-08	7.48164E-08	7.70609E-08
PC-3A	316	1.89	4161.42	-3845.222	3845.22	3737.831835	7.15749E-08	1.35276E-07	2.55673E-07
PC-3B	206	0.604	4031.19	-3824.993	3824.99	3696.805505	7.31723E-08	4.41961E-08	2.66944E-08
D1-2A	565	1.37	4108.76	-3544.263	3544.26	3721.24265	7.22144E-08	9.89338E-08	1.35539E-07
D1-2B	600	2.29	4201.93	-3601.528	3601.53	3750.592746	7.10886E-08	1.62793E-07	3.72796E-07
WLS Error Variance		234					SUM		1.80332E-06
							1.74485E-05		0.004438372

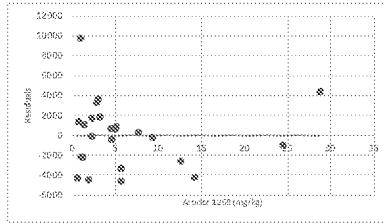
$$Var = \frac{\sum w_i}{((\sum w_i)(\sum w_i x_i^2) - (\sum w_i x_i)^2)}$$

WLS Var: OLS Var = 1.06  
Heteroscedasticity not severe

**Case 1a: Furan Congener Concentration and Aroclor 1268, Excluding Outliers (Co-location Study Data)**

Location	PCDD/F (ng/kg)	Aroclor 1268 (ng/kg)	Pred PCDD/F (ng/kg)	Pred PCDD/F*2	Residual PCDD/F	Residual*2
D1-1A	8114.0	2.29	6391.43	40850321.08	1722.57	2967262.60
D1-1B	8943.5	5.12	8042.13	64675853.13	901.37	812468.08
D1-2A	6944.9	1.37	5854.80	34278693.25	1090.10	1188316.11
D1-2B	6285.4	2.29	6391.43	40850321.08	-106.03	11241.43
D2-1A	10470.6	3.03	6823.06	46554127.52	3647.54	13304558.87
D2-1B	8782.1	3.22	6933.88	48078736.04	1848.22	3415905.39
EC-1A	8337.3	4.49	7674.66	58900384.83	662.64	439093.61
EC-1B	7319.9	4.58	7727.15	59708916.81	-407.25	165856.24
EC-2A	9803.0	12.6	12405.12	153887055.90	-2602.12	6771039.75
EC-2B	3760.2	5.67	8362.94	69938734.39	-4602.74	21185198.41
EC-4A	26257.2	28.8	21854.38	477614078.61	4402.82	19384793.04
EC-4B	9798.3	7.66	9523.68	99700494.85	274.62	75415.74
LC-1A	6838.7	0.721	5476.25	29989282.64	1362.45	1856277.82
LC-1B	15399.8	0.964	5617.99	31561767.27	9775.81	95566538.37
MC-1A	10308.4	9.35	10509.44	110448266.41	-201.04	40415.88
MC-1B	10940.3	2.86	6723.90	45210825.84	3316.40	10998511.61
MC-2A	8594.3	4.98	7960.47	63369076.32	633.83	401740.97
MC-2B	9115.8	14.2	13338.38	177912448.88	-4222.58	17830203.34
MC-3A	5032.9	5.68	8368.77	70936328.39	-3335.87	11128035.47
PC-1A	18360.8	24.5	19346.25	374277243.55	-985.45	971104.29
PC-2A	3534.4	1.24	5778.97	33396534.32	-2244.57	5038110.05
PC-2B	3473.3	1.03	5656.48	31995800.40	-2183.18	4766288.19
PC-3A	1691.0	1.89	6158.11	37922324.88	-4467.11	19955076.18
PC-3B	1127.6	0.604	5408.00	29246490.67	-4280.43	18322102.09

**Test for Zero Conditional Mean of Errors**



No discernable relationship between residuals and independent variable  
 $\text{Cov}(\hat{y}_i, x_i) = 0$

**Tests for Homoscedasticity**

BREUSCH-PAGAN SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.072209385
R Square	0.005214195
Adjusted R Square	-0.040093341
Standard Error	19958058.24
Observations	24

$$\hat{u}^2 = d_0 + xd_1$$

$H_0$  = homoscedasticity of residuals  
 $H_a$  = heteroscedasticity of residuals  
 $p > 0.05$   
**Status: Homoscedastic**

ANOVA

	df	SS	MS	F	Significance F
Regression	1	4.59322E+13	4.59322E+13	0.115313564	0.737394415
Residual	22	8.76313E+15	3.98324E+14		
Total	23	8.80906E+15			

Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%	
Intercept	11900180.61	5409827.908	2.199733672	0.038627995	680884.2063	23119477.01	680884.2063	23119477.01
Aroclor 1268 (ng/kg)	-194508.3516	572793.4665	-0.33957851	0.737394415	-1382409.295	993392.5921	-1382409.295	993392.5921

WHITE'S SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.252031857
R Square	0.063520957
Adjusted R Square	-0.025668509
Standard Error	19820035.55
Observations	24

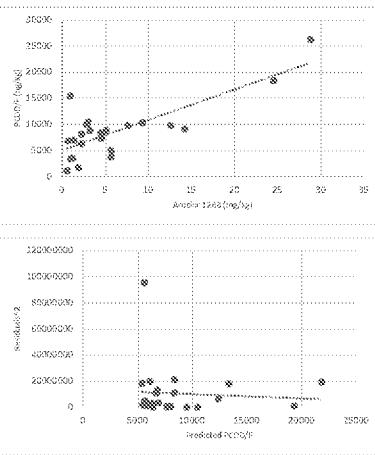
$$\hat{u}^2 = d_0 + \hat{Y} \times d_1 + \hat{Q}^2 \times d_2$$

$H_0$  = homoscedasticity of residuals  
 $H_a$  = heteroscedasticity of residuals  
 $p > 0.05$   
**Status: Homoscedastic**

ANOVA

	df	SS	MS	F	Significance F
Regression	2	5.59552E+14	2.79776E+14	0.712199555	0.502035056
Residual	21	8.24951E+15	3.92834E+14		
Total	23	8.80906E+15			

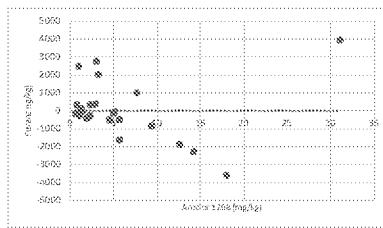
Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%	
Intercept	44901874.2	28949663.02	1.551032707	0.13583456	-1530245.82	10510594.2	-1530245.82	10510594.2
Pred PCDD/F (ng/kg)	-6507.035708	5486.446568	-1.186020064	0.248860625	-17916.72595	4902.654533	-17916.72595	4902.654533
Pred PCDD/F*2	0.240634362	0.210446219	1.143448255	0.265720578	0.197012509	0.678281233	0.197012509	0.678281233



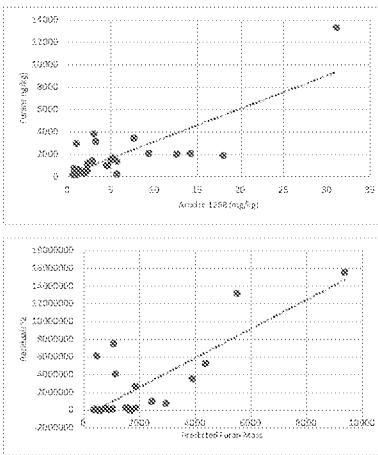
**Case 1b: Furan Congener Concentration and Aroclor 1268, Excluding Outliers (Co-location Study Data)**

Location	Furans (mg/kg)	Aroclor 1268 (mg/kg)	Pred PCDD/F (mg/kg)	Pred PCDD/F'2	Residual PCDD/F	Residual'2
D1-1A	1206.0	2.29	870.28	757380.79	335.72	112710.42
D1-1B	1641.0	5.12	1704.74	2906154.11	-63.74	4063.37
D1-2A	564.5	1.37	599.00	358801.42	-34.50	1190.27
D1-2B	600.4	2.29	870.28	757380.79	-269.88	72833.20
D2-1A	3831.0	3.03	1088.48	1184781.02	2742.52	7521435.33
D2-1B	3162.0	3.22	1144.50	1309882.18	2017.50	4070302.86
EC-1A	999.2	4.49	1518.98	2307298.89	-519.78	270170.79
EC-1B	1001.7	4.58	1545.52	2388624.09	-543.82	295737.38
EC-2A	2030.0	12.6	3910.34	15290725.74	-1880.34	3535662.56
EC-2B	229.9	5.67	1866.92	3485391.81	-1637.02	2679835.82
EC-4B	3446.0	7.66	2453.70	6020653.59	992.30	984655.29
LC-1A	728.2	0.721	407.63	166164.57	329.57	102763.28
LC-1B	2958.0	0.964	479.29	229714.22	2478.71	6144027.51
MC-1A	2089.0	9.35	2952.02	9714446.21	-863.02	744810.57
MC-1B	1409.0	2.86	1038.35	1978169.46	370.65	137381.87
MC-2A	1515.0	4.98	1663.46	2767110.71	-148.46	22941.40
MC-2B	2089.0	14.2	4382.12	19202975.39	-2293.12	5258399.18
MC-3A	1358.0	5.68	1869.87	3496410.30	-511.87	262009.93
MC-3B	1872.0	18	5502.61	30278688.84	-3630.61	13181310.52
PC-1A	13310.0	31.1	9365.34	87709605.64	3944.66	15569337.32
PC-2A	649.3	1.24	560.67	314348.48	88.63	7855.65
PC-2B	206.7	1.03	498.75	248747.78	-292.05	85290.99
PC-3A	316.2	1.89	752.33	566090.76	-436.13	190209.57
PC-3B	206.2	0.604	373.13	139228.73	-166.93	27866.85

Test for Zero Conditional Mean of Errors



No discernable relationship between residuals and independent variable  
 $\text{Cov}(\hat{u}_i, x_i) = 0$



Tests for Homoscedasticity

BREUSCH-PAGAN SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.796165103
R Square	0.633878871
Adjusted R Square	0.617237001
Standard Error	264227.972
Observations	24

$$\hat{u}^2 = d_0 + d_1 x_1$$

$H_0$  = homoscedasticity of residuals  
 $H_a$  = heteroscedasticity of residuals  
 $p < 0.05$   
**Status: Heteroscedastic**

ANOVA

	df	SS	MS	F	Significance F
Regression	1	2.65916E+14	2.65916E+14	38.0894028	3.2714E-06
Residual	22	1.5359E+14	6.98137E+12		
Total	23	4.19506E+14			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	-380393.2471	718892.6532	-0.529137758	0.602008656	-1871285.359	1110498.865	-1871285.359	1110498.865
Aroclor 1268 (mg/kg)	485737.7233	78704.53387	6.171661268	3.2714E-06	322514.5102	648960.9364	322514.5102	648960.9364

WHITE'S SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.815094063
R Square	0.664378331
Adjusted R Square	0.632414363
Standard Error	2589313.161
Observations	24

$$\hat{u}^2 = d_0 + \hat{Y} \times d_1 + d_2^2 \times d_2$$

$H_0$  = homoscedasticity of residuals  
 $H_a$  = heteroscedasticity of residuals  
 $p < 0.05$   
**Status: Heteroscedastic**

ANOVA

	df	SS	MS	F	Significance F
Regression	2	2.78711E+14	1.39355E+14	20.78522672	1.05057E-05
Residual	21	1.40795E+14	6.70454E+12		
Total	23	4.19506E+14			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	388910.5307	1082050.564	0.360344094	0.722188873	-1860336.804	2640157.865	-1860336.804	2640157.865
Pred PCDD/F (mg/kg)	590.4088742	808.5613121	0.730196789	0.473337784	-1091.086425	2271.904173	-1091.086425	2271.904173
Pred PCDD/F'2	0.124786249	0.09030383	1.381435869	0.18166771	-0.063066996	0.312639493	-0.063066996	0.312639493

Location	PCDD/F (mg/kg)	Aroclor 1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight	Weight * X	Weight * X^2
D1-1A	1206.0	2.29	870.28	335.724	335.72	646.0334516	2.39602E-06	5.48688E-06	1.2565E-05
D1-1B	1641.0	5.12	1704.74	-63.745	63.74	994.4479433	1.0112E-06	5.17733E-06	2.65079E-05
D1-2A	564.5	1.37	599.00	-34.500	34.50	532.7679632	3.52309E-06	4.82663E-06	6.61249E-06
D1-2B	600.4	2.29	870.28	-269.876	269.88	646.0334516	2.39602E-06	5.48688E-06	1.2565E-05
D2-1A	3831.0	3.03	1088.48	2742.524	2742.52	737.1383011	1.84036E-06	5.57628E-06	1.68961E-05
D2-1B	3162.0	3.22	1144.50	2017.499	2017.50	760.5300867	1.72889E-06	5.56702E-06	1.79258E-06
EC-1A	999.2	4.49	1518.98	-519.780	519.78	916.8857067	1.18951E-06	5.34092E-06	2.39807E-05
EC-1B	1001.7	4.58	1545.52	-534.817	534.82	927.9660262	1.16128E-06	5.31865E-06	2.43594E-05
EC-2A	2030.0	12.6	3910.34	-1880.336	1880.34	1915.34561	2.72587E-07	3.4346E-06	4.3276E-05
EC-2B	229.9	5.67	1866.92	-1637.020	1637.02	1062.161007	8.83379E-07	5.02577E-06	2.84946E-05
EC-4B	3446.0	7.66	2453.70	992.298	992.30	1307.159183	5.85252E-07	4.48303E-06	3.434E-05
LC-1A	728.2	0.721	407.63	320.567	320.57	452.866548	4.87595E-06	3.51556E-06	2.53472E-06
LC-1B	2958.0	0.964	479.29	2478.715	2478.71	482.7834107	4.29038E-06	4.13592E-06	3.98703E-06
MC-1A	2089.0	9.35	2952.02	-863.024	863.02	1515.22961	4.35559E-07	4.07248E-06	3.80776E-05
MC-1B	1409.0	2.86	1038.35	370.651	370.65	716.2088086	1.94949E-06	5.57554E-06	1.5946E-05
MC-2A	1515.0	4.98	1663.46	-148.463	148.46	977.2118907	1.04718E-06	5.21497E-06	2.59706E-05
MC-2B	2089.0	14.2	4382.12	-2293.120	2293.12	2112.329069	2.24118E-07	3.18248E-06	4.51912E-05
MC-3A	1358.0	5.68	1869.87	-511.869	511.87	1063.392154	8.84327E-07	5.02298E-06	2.85305E-05
MC-3B	1872.0	18	5502.61	-3630.607	3630.61	2580.164782	1.50212E-07	2.70382E-06	4.86687E-05
PC-1A	13310.0	31.1	9365.34	3944.659	3944.66	4192.966846	5.68797E-08	1.76896E-06	5.50146E-05
PC-2A	649.3	1.24	560.67	88.632	88.63	516.7630572	3.7447E-06	4.64343E-06	5.75785E-06
PC-2B	206.7	1.03	498.75	-292.046	292.05	490.9308783	4.14952E-06	4.27401E-06	4.40223E-06
PC-3A	316.2	1.89	752.33	-436.130	436.13	596.7875871	2.80776E-06	5.30667E-06	1.00296E-05
PC-3B	206.2	0.604	373.13	-166.934	166.93	438.4621326	5.20159E-06	3.14176E-06	1.89762E-06

$$\text{WLS Error Variance} = 3533 \quad \text{Var} = \frac{\sum w_i}{(\sum w_i)(\sum w_i x_i^2) - (\sum w_i x_i)^2}$$

Case 1b: Furan Congener Concentration and Aroclor 1268, Excluding Outliers (Co-location Study Data)

Location Furan (mg/kg) Aroclor 1268 (mg/kg)

Location	Furan (mg/kg)	Aroclor 1268 (mg/kg)
D1-1A	120.0	2.29
D1-1B	1641.0	5.32
D1-2A	564.5	1.37
D1-2B	600.4	2.29
D2-1A	3831.0	3.03
D2-1B	3162.0	3.22
EC-1A	999.2	4.49
EC-1B	505.7	4.56
EC-2A	2030.0	3.26
EC-2B	238.9	5.67
EC-4B	3406.0	7.66
LC-1A	728.2	0.723
LC-1B	2998.0	0.964
MC-1A	2089.0	9.35
MC-1B	1409.0	2.86
MC-2A	1515.0	4.98
MC-2B	2089.0	14.2
MC-3A	1358.0	5.68
MC-3B	1872.0	18
PC-1A	3131.0	311.1
PC-2A	649.3	1.34
PC-2B	205.7	1.03
PC-3A	316.2	1.89
PC-3B	205.2	0.604

Weighted Least Squares performed with "Real Stats" Add-in

$$Pred Y'_i = Abs(Res)x + \hat{\sigma}_1$$

$$W_i = \frac{1}{Pred Y'_i^2}$$

WLS solution is asymptotic at iteration #4.

Iteration #1 Location Y: Furan (mg/kg) X: Aroclor 1268 (mg/kg) Pred Y Residual Aroclor 1268 Pred Y Weight

Location	Y: Furan (mg/kg)	X: Aroclor 1268 (mg/kg)	Pred Y	Residual	Aroclor 1268	Pred Y	Weight
D1-1A	120.0	2.29	8.70E+02	3.36E+02	6.40E+02	2.40E-06	
D1-1B	1641.0	5.32	1.70E+03	-6.71E+02	9.41E+02	1.80E-06	
D1-2A	564.5	1.37	5.99E+02	3.61E+03	5.53E+02	3.93E-06	
D1-2B	600.4	2.29	8.70E+02	-2.70E+02	6.05E+02	2.40E-06	
D2-1A	3831.0	3.03	1.09E+03	-2.74E+03	7.37E+02	1.94E-06	
D2-1B	3162.0	3.22	1.14E+03	-2.02E+03	7.51E+02	1.71E-06	
EC-1A	999.2	4.49	1.52E+03	-5.20E+02	9.17E+02	1.19E-06	
EC-1B	1001.7	4.58	1.53E+03	-5.44E+02	9.28E+02	1.16E-06	
EC-2A	2030.0	12.6	3.91E+03	-1.88E+03	1.92E+03	2.73E-07	
EC-2B	229.9	5.67	1.97E+03	-1.64E+03	1.64E+03	1.05E-07	
EC-4B	3406.0	7.66	2.45E+03	-9.94E+02	1.31E+03	5.93E-07	
LC-1A	728.2	0.723	4.02E+02	3.20E+02	4.02E+02	4.90E-06	
LC-1B	2998.0	0.964	4.79E+02	2.48E+03	4.80E+02	4.95E-06	
MC-1A	2089.0	9.35	2.95E+03	-8.63E+02	8.61E+02	1.52E+03	4.88E-07
MC-1B	1409.0	2.86	1.04E+03	3.71E+02	7.35E+02	1.95E-06	
MC-2A	1515.0	4.98	1.68E+03	-1.49E+03	9.77E+02	1.05E-06	
MC-2B	2089.0	14.2	4.38E+03	-2.96E+03	2.11E+03	2.24E-07	
MC-3A	1358.0	5.68	1.87E+03	-5.12E+02	5.12E+02	1.05E-07	
MC-3B	1872.0	18	5.50E+03	-3.63E+03	3.63E+03	1.50E-07	
PC-1A	3131.0	311.1	9.37E+03	-3.94E+03	4.19E+03	5.69E-08	
PC-2A	649.3	1.24	5.61E+02	8.98E+01	5.17E+02	3.74E-06	
PC-2B	205.7	1.03	4.99E+02	-2.92E+02	2.92E+02	4.13E-06	
PC-3A	316.2	1.89	7.52E+02	-4.36E+02	5.97E+02	2.21E-06	
PC-3B	205.2	0.604	3.73E+02	-3.67E+02	1.67E+02	5.30E-06	

OVERALL FIT

Multiple R	0.610192021
R Square	0.368257988
Adjusted R Square	0.312029529
Standard Error	1.530570973
Observations	24

ANOVA							
	df	SS	MS	F	p-value	0.05	
Regression	3	10.42597488	3.41661708	4.65050946	0.046497196	yes	
Residual	22	51.53824508	2.342647504				
Total	23	61.95421998					

	coefficient	std. error	t stat	p-value	lower	upper	vif
Intercept	73.2303125	2.39148702	3.19125334	0.026166107	95.32269532	1309.30773	
X:Aroclor 1268 (mg/kg)	191.9261923	10.97651481	2.109623061	0.046497196	5.252409773	350.5998949	1

Iteration #2 Location Y: Furan (mg/kg) X: Aroclor 1268 (mg/kg) Pred Y Residual Aroclor 1268 Pred Y Weight

Location	Y: Furan (mg/kg)	X: Aroclor 1268 (mg/kg)	Pred Y	Residual	Aroclor 1268	Pred Y	Weight
D1-1A	120.0	2.29	1.18E+03	-4.51E+02	5.45E+02	3.10E-06	
D1-1B	1641.0	5.32	1.74E+03	-9.79E+01	9.81E+01	1.04E-06	
D1-2A	564.5	1.37	9.73E+02	-4.08E+02	4.23E+02	5.59E-06	
D1-2B	600.4	2.29	1.15E+03	-5.60E+02	5.60E+02	5.06E-06	
D2-1A	3831.0	3.03	1.31E+03	-2.52E+03	6.71E+02	2.22E-06	
D2-1B	3162.0	3.22	1.35E+03	-1.81E+03	6.98E+02	2.05E-06	
EC-1A	999.2	4.49	1.61E+03	-6.11E+02	6.11E+02	8.89E-07	
EC-1B	1001.7	4.58	1.63E+03	-6.27E+02	6.27E+02	1.27E-06	
EC-2A	2030.0	12.6	3.27E+03	-1.44E+03	1.44E+03	1.35E-06	
EC-2B	229.9	5.67	1.89E+03	-6.63E+02	6.63E+02	1.05E-07	
EC-4B	3406.0	7.66	2.36E+03	-1.39E+03	1.39E+03	5.39E-07	
LC-1A	728.2	0.723	8.24E+02	-1.12E+02	1.12E+02	9.35E-06	
LC-1B	2998.0	0.964	8.90E+02	-2.07E+02	3.83E+02	7.61E-06	
MC-1A	2089.0	9.35	2.60E+03	-8.54E+02	8.54E+02	3.84E-07	
MC-1B	1409.0	2.86	1.28E+03	-1.32E+02	6.05E+02	2.40E-06	
MC-2A	1515.0	4.98	1.71E+03	-1.95E+02	9.62E+02	1.08E-06	
MC-2B	2089.0	14.2	3.59E+03	-1.00E+03	1.00E+03	1.67E-07	
MC-3A	1358.0	5.68	1.87E+03	-4.54E+02	4.54E+02	1.05E-07	
MC-3B	1872.0	18	4.37E+03	-2.50E+03	2.50E+03	1.23E-07	
PC-1A	3131.0	311.1	7.05E+03	-6.80E+03	6.80E+03	3.40E-07	
PC-2A	649.3	1.24	9.48E+02	-2.39E+02	2.39E+02	6.04E-06	
PC-2B	205.7	1.03	9.03E+02	-6.97E+02	3.72E+02	7.21E-06	
PC-3A	316.2	1.89	1.08E+03	-7.68E+02	7.68E+02	5.01E-06	
PC-3B	205.2	0.604	8.16E+02	-6.10E+02	3.09E+02	1.05E-05	

OVERALL FIT

Multiple R	0.368345459
R Square	0.134295399
Adjusted R Square	0.098564187
Standard Error	1.81309562
Observations	24

ANOVA							
	df	SS	MS	F	p-value	0.05	
Regression	1	11.35833262	11.35833262	3.41024663	0.078209075	no	
Residual	22	73.74272712	3.330649733				
Total	23	84.53265073					

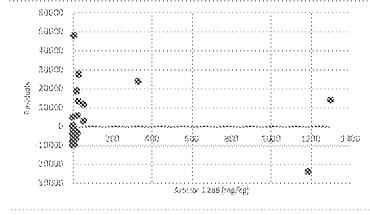
	coefficient	std. error	t stat	p-value	lower	upper	vif
Intercept	701.3884057	237.9862985	2.53269805	0.027384077	28.32122039	132.351776	1
X:Aroclor 1268 (mg/kg)	205.1227377	1.342669329	154.22277309	0.000126511	247.70629504	32.73127776	1

	Location	Furan (mg/kg)	Aroclor 1268 (mg/kg)	Pred Y	Residual	Aroclor 1268	Pred Y	Weight
D1-1A	120.0	2.29	112.39	43.00E	43.61	505.930176	5.23341E-06	7.38169E-06
D1-1B	1641.0	5.32	173.37	-93.372	93.37	981.0171036	1.03907E-06	5.365E-06
D1-2A	564.5	1.37	97.45	-101.953	41.98	516.9304176	5.69426E-06	7.79886E-06
D1-2B	600.4	2.29	116.39	-53.995	56.194	505.9304176	7.38136E-06	1.08041E-06
D2-1A	3831.0	3.03	311.96	-26.001	251.954	821.5295207	2.4197E-06	6.79317E-06
D2-1B	3162.0	3.22	310.59	-16.001	300.594	805.0295207	2.0293E-06	5.0293E-06
EC-1A	999.2	4.49	1087.04	-200.98	707.04	886.6024042	5.7117E-06	5.7117E-06
EC-1B	1001.7	4.58	1085.53	-62.532	523.533	920.1559398	1.2442E-06	5.653E-06
EC-2A	2030.0	12.6	126.37	-121.172	126.167	2101.292514	2.26371E-07	5.39180E-06
EC-2B	229.9	5.67	1845.53	-3615.634	2455.58	1053.427107	8.64269E-07	5.01351E-06
EC-4B	3446.0	7.66	2247.74	139.262	139.262	3361.601167	5.39387	

**Case 2a: PCDD/F Concentration and Aroclor 1268, Excluding Outliers (Cumulative Data Set)**

Location	PCDD/F (ng/kg)	Aroclor 1268 (mg/kg)	Pred PCDD/F (ng/kg)	Pred PCDD/F/P2	Residual PCDD/F	Residual P2
36	27038	55	15448.22	23867459.34	11589.68	13432070.24
61	141906	1300	12807.65	1638595962.71	13898.34	193163962.84
68	64192	330	40310.74	1624956138.98	23881.25	570314307.62
1718	18409	56	15538.63	21448954.90	2870.57	8240185.27
BR048	2981	1.4	10602.29	112408474.65	-7621.29	58084004.66
C-15	10834	0.099	10484.66	10992817.80	349.34	122035.65
C-6	59189	7.58	11161.02	124568257.20	48027.98	2306687255.47
C-8	10654	2.2	10674.61	113947376.41	-20.21	408.59
111	9396	6.1	11027.21	121599348.62	-1630.84	2659647.15
EPA-F2	94088	1188	117881.83	138961249.06	-23794.13	566160433.26
GRID MARSH	5980	6.1	11027.21	121599348.62	-5047.21	25474324.52
117	2133	11	11470.21	131565820.13	-9336.80	87175852.47
110	3049	0.25	10498.32	110215633.17	-7449.72	55496264.46
100	856	1.1	10575.16	111834083.85	-9719.46	94467911.47
101	2058	0.085	10483.40	109901638.12	-8425.80	70994176.66
102	2678	0.13	10487.47	109986956.27	-7809.45	60987503.49
D1-1A	8114	2.29	10682.75	114121157.58	-2568.75	6598478.97
D1-1B	8944	5.12	10998.61	119653155.14	-1995.11	3980457.78
D1-2A	6945	1.37	10599.57	112350969.36	-3654.67	13356642.18
D1-2B	6285	2.29	10682.75	114121157.58	-4397.35	19336691.15
D2-1A	10471	3.03	10749.65	115555045.35	-279.05	77870.73
D2-1B	8782	3.22	10766.83	115924650.03	-1984.73	393915.719
EC-1A	8337	4.49	10881.65	118410321.47	-2544.35	6473720.37
EC-1B	7320	4.58	10889.79	118587471.89	-3569.89	12744096.79
EC-2A	9803	12.6	11614.87	134905185.91	-1811.87	3282869.90
EC-2B	3760	5.67	10988.33	120743473.47	-7228.13	52245914.13
EC-3A	9344	24.4	12681.70	160825453.11	-3338.00	1114227.74
EC-3B	31228	22.1	12473.76	155594599.66	-18754.64	351736655.16
EC-4A	26257	28.8	13079.50	171073267.44	-13177.70	173651830.49
EC-4B	9798	7.66	11168.25	124729758.83	-1369.95	1876756.36
LC-1A	6839	0.721	10540.90	11110540.27	-370.20	13706273.41
LC-1B	15394	0.964	10562.87	111574178.03	4830.93	23337905.06
MC-1A	10308	9.35	11321.04	128165931.28	-1012.64	1925438.39
MC-1B	10040	2.86	10734.28	115224846.65	-691.98	481613.38
MC-2A	8594	4.98	10925.95	119376409.15	-2331.65	5436597.22
MC-2B	9116	14.2	11759.52	138286401.66	-2643.72	6989275.90
MC-3A	5033	5.68	10989.24	120763343.21	-5956.34	35477957.71
MC-3B	6018	18	12103.08	146484515.86	-6084.78	37024532.75
PC-1A	40766	31.1	13287.44	176556098.06	27478.86	755087795.90
PC-1B	18361	24.5	12690.74	161054843.24	5670.06	32149597.61
PC-2A	3534	1.24	10587.82	112101949.80	-7053.42	49750745.32
PC-2B	3473	1.03	10568.83	111703271.04	-7095.53	50346615.45
PC-3A	1691	1.89	10646.59	113349810.38	-8955.59	8020534.84
PC-3B	1128	0.604	10530.32	110887651.56	-9402.75	88411718.50

Test for Zero Conditional Mean of Errors



No discernable relationship between residuals and independent variable  
 $\text{Cov}(\hat{u}_i, x_i) = 0$

Tests for Homoscedasticity

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.174021468
R Square	0.030283471
Adjusted R Square	0.007194983
Standard Error	371182846.5
Observations	44

$$\hat{u}^2 = d_0 + x_1 d_1$$

$H_0$  = homoscedasticity of residuals  
 $H_a$  = heteroscedasticity of residuals  
 $p < 0.05$   
**Status: Homoscedastic**

ANOVA

	df	SS	MS	F	Significance F
Regression	1	1.80712E+17	1.80712E+17	1.311626403	0.258584621
Residual	42	5.78662E+18	1.37777E+17		
Total	43	5.96733E+18			

Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%	
Intercept	120107474.9	58109806.81	2.066905424	0.044943247	2837137	237377812.8	2837137	237377812.8
Aroclor 1268 (mg/kg)	245964.9515	214767.2974	1.145262591	0.258584621	-187453.0017	679382.9048	-187453.0017	679382.9048

WHITE'S SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.26801126
R Square	0.071830036
Adjusted R Square	0.026553452
Standard Error	367546228.8
Observations	44

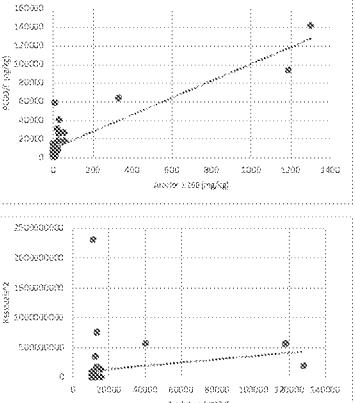
$$\hat{u}^2 = d_0 + \hat{Y} \times d_1 + \hat{Y}^2 \times d_2$$

$H_0$  = homoscedasticity of residuals  
 $H_a$  = heteroscedasticity of residuals  
 $p < 0.05$   
**Status: Homoscedastic**

ANOVA

	df	SS	MS	F	Significance F
Regression	2	4.28634E+17	2.14317E+17	1.586472073	0.216952154
Residual	41	5.5387E+18	1.3509E+17		
Total	43	5.96733E+18			

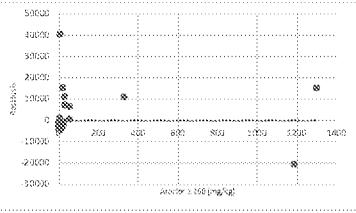
Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%	
Intercept	-176807270.7	209618824	-0.843470468	0.403859668	-600141033.5	246526492.1	-600141033.5	246526492.1
Pred PCDD/F (ng/kg)	27879.9853	18720.20042	1.489299509	0.144061262	.9926.226419	65686.19701	.9926.226419	65686.19701
Pred PCDD/F/P2	-0.190333336	0.140497673	-1.354708106	0.1829899	-0.474074142	0.09340747	-0.474074142	0.09340747



**Case 2b: Furan Congener Concentration and Aroclor 1268, Excluding Outliers (Cumulative Data Set)**

Location	Furans (ng/kg)	Aroclor 1268 (mg/kg)	Pred PCDD/F (ng/kg)	Pred PCDD/F <sup>2</sup>	Residual PCDD/F	Residual PCDD/F <sup>2</sup>
36	14468	55	8046.63	64748193.11	6421.37	41234040.54
61	122400	1300	107225.33	11497271349.46	15174.67	230270580.31
68	40850	330	29953.57	897216281.25	10896.43	118732193.34
1718	8750	56	8126.29	66036553.47	623.71	389016.95
BR048	391	1.4	3776.76	14263945.82	-3385.76	11463397.41
C-15	1348	0.099	3673.12	13491841.25	2325.12	54062024.43
C-6	44710	7.58	4269.07	18224981.55	40440.93	1635468568.49
C-8	2826	2.2	3804.09	14749388.19	-1014.49	1029196.54
111	5036	6.1	4151.17	17232241.42	884.91	783061.29
EPA-F2	77700	1188	98303.23	9663524940.08	-20603.23	244493067.91
GRID MARSH	3690	6.1	4151.17	17232241.42	-461.17	212681.07
117	148	11	4541.52	20625361.99	-4393.91	19306422.10
110	639	0.25	3685.15	13580353.25	-305.15	9333960.37
100	71	1.1	3752.87	14083999.10	-3682.37	13559815.32
101	161	0.985	3672.01	13483649.50	-3510.91	12326488.46
102	147	0.13	3675.59	13509988.98	-3528.24	12448489.43
D1-1A	1206	2.29	3847.66	14804508.77	2641.66	6978382.18
D1-1B	1641	5.12	4073.11	16590185.33	-2432.11	5915135.32
D1-2A	565	1.37	3774.37	14245899.75	-3209.87	10391291.65
D1-2B	600	2.29	3847.66	14804508.77	-3247.26	10544715.48
D2-1A	3831	3.03	3906.61	15261620.12	-75.61	5717.23
D2-1B	3162	3.22	3921.75	15380107.88	-759.75	577217.12
EC-1A	999	4.49	4022.92	16183871.71	-3023.72	9142872.40
EC-1B	1002	4.58	4030.09	16241608.10	-3028.39	9171132.99
EC-2A	2030	12.6	4668.97	21799317.83	-2638.97	6964183.56
EC-2B	239	5.67	4116.92	16949022.11	-3887.02	15108916.76
EC-3A	3810	24.4	5608.98	31460667.29	-1798.98	3236324.26
EC-3B	20737	22.1	5425.76	29438863.41	15311.24	2344340993.37
EC-4A	17065	28.8	5959.49	35515545.26	11105.51	123332307.27
EC-4B	3446	7.66	4275.45	18279435.16	-829.45	687980.02
LC-1A	728	0.721	3722.67	13858299.49	-2994.47	8966872.25
LC-1B	2958	0.964	3742.03	14027995.55	-784.03	614705.35
MC-1A	2089	9.35	4140.07	19448750.29	-2321.07	5387383.26
MC-1B	1409	2.86	3893.07	15155993.13	-2484.07	6170603.19
MC-2A	1515	4.98	4061.95	16499458.08	-2546.95	6486967.02
MC-2B	2089	14.2	4796.43	2305765.05	-2797.43	7330190.93
MC-3A	1358	5.68	4117.72	16955581.95	-2759.72	7616030.32
MC-3B	1872	18	5099.15	26001296.55	-3227.15	10414475.50
PC-1A	13310	31.1	6142.71	37732931.99	7167.29	51369992.45
PC-1B	4611	24.5	5616.95	31550094.84	-1005.95	1011929.59
PC-2A	649	1.24	3764.02	14167832.09	-3114.72	9701468.70
PC-2B	207	1.03	3747.29	14042175.89	-3540.59	12353771.45
PC-3A	316	1.89	3815.80	14560315.32	-3499.60	12247187.03
PC-3B	206	0.604	3713.35	13788992.69	-3507.15	12300124.23

Test for Zero Conditional Mean of Errors



No discernable relationship between residuals and independent variable  
 $\text{Cov}(\hat{u}_t, x_t) = 0$

Tests for Homoscedasticity

BREUSCH-PAGAN SUMMARY OUTPUT	
Regression Statistics	
Multiple R	0.222572919
R Square	0.049538704
Adjusted R Square	0.026908673
Standard Error	250707407.7
Observations	44

$$\hat{u}^2 = d_0 + d_1 x_1$$

$H_0$  = homoscedasticity of residuals  
 $H_A$  = heteroscedasticity of residuals  
 $p < 0.05$   
**Status: Homoscedastic**

ANOVA

	df	SS	MS	F	Significance F
Regression	1	1.37592E+17	1.37592E+17	2.189069229	0.146455485
Residual	42	2.63988E+18	6.28542E+16		
Total	43	2.77747E+18			

Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%	
Intercept	55366728.76	39249099.38	1.410642705	0.165714062	-23841378.93	134574036.5	-23841378.93	134574036.5
Aroclor 1268 (mg/kg)	214623.4484	145059.9156	1.479550347	0.146455485	-78119.31305	507366.2099	-78119.31305	507366.2099

$H_0$  = homoscedasticity of residuals  
 $H_A$  = heteroscedasticity of residuals  
 $p < 0.05$   
**Status: Homoscedastic**

WHITE'S SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.224546383
R Square	0.050421078
Adjusted R Square	0.004100155
Standard Error	253628584.5
Observations	44

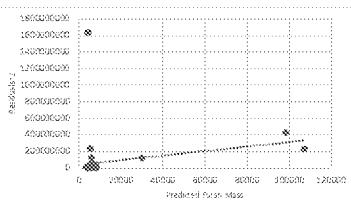
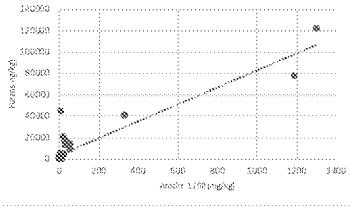
$$\hat{u}^2 = d_0 + \hat{Y} \times d_1 + \hat{Y}^2 \times d_2$$

$H_0$  = homoscedasticity of residuals  
 $H_A$  = heteroscedasticity of residuals  
 $p < 0.05$   
**Status: Homoscedastic**

ANOVA

	df	SS	MS	F	Significance F
Regression	2	1.40043E+17	7.00215E+16	1.088516264	0.346247663
Residual	41	2.63743E+18	6.43275E+16		
Total	43	2.77747E+18			

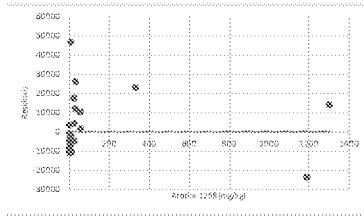
Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%	
Intercept	33848764	72970227.03	0.463867709	0.645195998	-113518608.9	181216136.9	-113518608.9	181216136.9
Pred PCDD/F (mg/kg)	5261.840147	13283.13063	0.396129519	0.694063569	-21563.98637	32087.66666	-21563.98637	32087.66666
Pred PCDD/F <sup>2</sup>	-0.024374462	0.124876961	-0.195187824	0.84620999	-0.276568601	0.227819676	-0.276568601	0.227819676



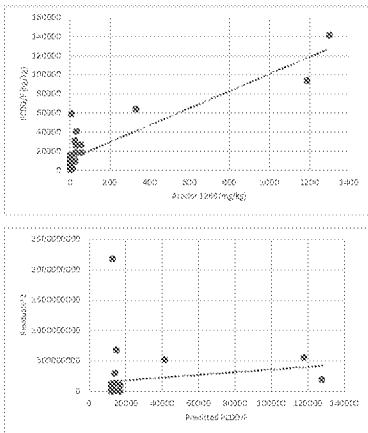
**Case 3a: PCDD/F Concentration and Aroclor 1268, Excluding Outliers (Original Distribution)**

Location	PCDD/F (ng/kg)	Aroclor 1268 (mg/kg)	Pred PCDD/F (ng/kg)	Pred PCDD/F^2	Residual PCDD/F	Residual^2
36	27038	55	16744.67	280384012.67	10293.23	105950556.47
61	141906	1300	127780.77	1632792642.81	14125.22	195921946.69
68	64192	330	41270.72	170322179.76	22921.28	525385115.12
1718	18409	56	16833.86	283378734.69	1575.34	2481706.59
BR048	2981	1.4	11964.32	143144992.42	-8983.32	8079067.65
C-15	10834	0.099	11848.29	140382003.08	-1014.29	1028786.62
C-6	50189	7.58	12515.49	156637460.17	46673.51	2178416567.24
111	9396	6.1	12383.49	153350925.75	-2987.13	8922928.22
EPA-F2	94088	1188	117791.98	13874951701.26	-23704.28	561893121.53
GRID MARSH	5980	6.1	12383.49	153350925.75	-6403.49	41004237.92
117	2133	11	128020.50	164365313.84	-10687.09	114213895.87
110	3049	0.25	11861.76	140701307.02	-8813.16	77671257.03
100	856	1.1	11937.57	142506480.98	-11081.87	122807753.10
101	2058	0.098	11847.04	140352417.12	-9789.45	95833302.86
102	2678	0.13	11851.06	140447525.96	-9173.04	8414642.67
D2-1A	10471	3.03	12109.69	146644693.97	-1639.09	2686629.84
D2-1B	8782	3.22	12126.64	14705385.16	-334.54	11185944.36
EC-3A	9344	24.4	14015.59	196436791.97	-4671.89	21826565.81
EC-3B	31228	22.1	13810.46	1907288918.47	17417.94	303384491.26
EC-4A	26257	28.8	14408.01	207590688.30	11849.19	140403356.17
EC-4B	9798	7.66	12522.62	156816103.35	-3724.32	7421939.41
LC-1A	6839	0.721	11903.76	141699611.78	-5065.06	25654879.46
LC-1B	15394	0.964	11925.44	142216940.78	3468.36	12029543.90
PC-1A	40766	31.1	14613.13	213543706.42	26153.17	689388954.02
PC-1B	18361	24.5	14024.51	196686869.36	4336.29	18803414.48
PC-2A	3534	1.24	11950.05	142803741.49	-8415.65	70823197.66
PC-2B	3473	1.03	11931.32	142356467.66	-8458.02	71538152.45
PC-3A	1691	1.89	12008.02	144192606.80	-10317.02	106440955.36
PC-3B	1128	0.604	11893.33	141451295.80	-10765.76	115901585.95
D1-2A	6945	1.37	11961.65	143080976.85	-5016.75	25167741.19
D1-2B	6285	2.29	12043.70	140505633.85	-5758.30	33157982.63

Test for Zero Conditional Mean of Errors



No discernable relationship between residuals and independent variable  
 $\text{Cov}(\hat{u}_i, x_i) = 0$



Tests for Homoscedasticity

BREUSCH-PAGAN SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.150080547
R Square	0.022524171
Adjusted R Square	-0.011181892
Standard Error	408917639.9
Observations	31

$$\hat{u}^2 = d_0 + x d_1$$

$H_0$  = homoscedasticity of residuals

$H_A$  = heteroscedasticity of residuals

p>0.05

Status: Homoscedastic

ANOVA

	df	SS	MS	F	Significance F
Regression	1	1.11741E+17	1.11741E+17	0.668252787	0.420327161
Residual	29	4.8492E+18	1.67214E+17		
Total	30	4.96094E+18			

Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	165003086.7	77303783.54	2.186220117	0.03701769	1089097.13	327107076.2	1089097.13
Aroclor 1268 (mg/kg)	156068.666	23984.9407	0.8174673	0.420327161	-294477.4972	686614.8292	-294477.4972

WHITE'S SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.228677037
R Square	0.052293187
Adjusted R Square	-0.015400156
Standard Error	409769676.2
Observations	31

$$\hat{u}^2 = d_0 + \hat{Y} \times d_1 + \hat{Y}^2 \times d_2$$

$H_0$  = homoscedasticity of residuals

$H_A$  = heteroscedasticity of residuals

p<0.05

Status: Homoscedastic

ANOVA

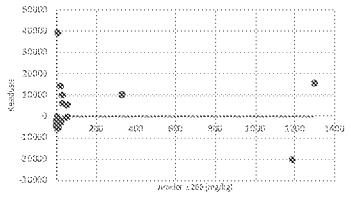
	df	SS	MS	F	Significance F
Regression	2	2.59423E+17	1.29712E+17	0.772501171	0.47145043
Residual	28	4.70151E+18	1.67911E+17		
Total	30	4.96094E+18			

Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%	
Intercept	-101048245.6	276161511.7	-0.36550271	0.71187736	-666739458.6	464642967.3	-666739458.6	464642967.3
Pred PCDD/F (ng/kg)	22545.33849	21862.45551	1.03123542	0.31125627	-22237.87152	67326.5485	-22237.87152	67328.5485
Pred PCDD/F^2	-0.152167302	0.162254624	-0.937830299	0.356351349	-0.484530832	0.180196228	-0.484530832	0.180196228

**Case 3b: Furan Congener Concentration and Aroclor 1268, Excluding Outliers (Original Distribution)**

Location	Furans (ng/kg)	Ar1268 (mg/kg)	Pred PCDD/F (ng/kg)	Pred PCDD/F <sup>2</sup>	ResiduePCDD/F	ResidueP <sup>2</sup>
36	14468	55	9217.10	84954884.02	5250.90	27571977.55
61	122400	1300	107010.60	11451268613.06	15389.40	236833581.83
68	40850	330	30818.07	94973558.99	100319.93	100639561.43
1718	8750	56	9295.65	86409041.50	-545.65	29777.92
BR048	391	1.4	5006.87	25068757.78	-4615.87	21306265.60
C-15	1348	0.099	4904.68	24055874.23	-3556.68	12649964.12
C-6	44710	7.58	5492.30	30165401.78	39217.70	1538027656.97
111	5036	6.1	5376.05	28901928.12	-339.97	115579.84
EPA-F2	77700	1188	98213.11	9645815494.80	-20513.11	420787790.26
GRID MARSH	3690	6.1	5376.05	28901928.12	-1686.05	2842769.41
117	148	11	5760.94	33188446.30	-5613.33	31509512.34
110	630	0.25	4916.54	24172362.71	-4286.54	18374422.68
100	71	1.1	4983.31	24833342.25	-4912.81	24135666.31
101	161	0.085	4903.58	24045088.23	-4742.48	22491117.73
102	147	0.13	4907.11	24079766.13	-4759.76	22655332.67
D2-1A	3831	3.03	5134.91	26367258.86	-1303.91	1709170.66
D2-1B	3162	3.22	5149.83	26520751.44	-1987.83	3951469.04
EC-3A	3810	24.4	6813.50	46423755.30	-3003.50	9021000.37
EC-3B	20737	22.1	6632.84	43994504.46	14104.16	198927461.16
EC-4A	17065	28.8	7159.11	51252907.76	9905.89	98126585.07
EC-4B	3446	7.66	5498.59	30234467.66	-2052.59	4213116.63
LC-1A	728	0.721	4953.54	24537521.75	-4225.34	17853466.74
LC-1B	2958	0.964	4972.62	24726986.40	-2014.62	4058708.63
PC-1A	13310	31.1	7339.78	53872316.31	5970.22	35643570.89
PC-1B	4611	24.5	6821.35	46530855.68	-2210.35	4885660.04
PC-2A	649	1.24	4994.30	24943364.63	-4345.00	18879052.96
PC-2B	207	1.03	4977.81	24778571.77	-4771.11	22763470.86
PC-3A	316	1.89	5045.36	25455658.20	-4729.16	22364954.93
PC-3B	206	0.604	4944.35	24446557.91	-4738.15	22450028.03
D1-2A	565	1.37	5004.51	25045166.25	-4440.01	19713729.54
D1-2B	600	2.29	5076.78	25773691.78	-4476.38	20037974.91

Test for Zero Conditional Mean of Errors



No discernable relationship between residuals and independent variable  
 $\text{Cov}(\hat{u}, x) = 0$

Tests for Homoscedasticity

BREUSCH-PAGAN SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.214209487
R Square	0.045885704
Adjusted R Square	0.012985211
Standard Error	279788694.1
Observations	31

$$\hat{u}^2 = d_0 + x d_1$$

$H_0$  = homoscedasticity of residuals  
 $H_a$  = heteroscedasticity of residuals  
 $p < 0.05$

Status: Homoscedastic

ANOVA

	df	SS	MS	F	Significance F
Regression	1	1.09178E+17	1.09178E+17	1.394681365	0.247211408
Residual	29	2.27017E+18	7.82817E+16		
Total	30	2.37935E+18			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	76793059.1	52892618.3	1.451867228	0.157272254	-31384491.7	184970609.9	-31384491.7	184970609.9
Ar1268 (mg/kg)	193807.0716	164108.8947	1.180966285	0.247211408	-141833.3043	529447.4475	-141833.3043	529447.4475

WHITE'S SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.214211012
R Square	0.045883518
Adjusted R Square	-0.022264617
Standard Error	284740993.4
Observations	31

$$\hat{u}^2 = d_0 + \hat{Y} \times d_1 + \hat{Y}^2 \times d_2$$

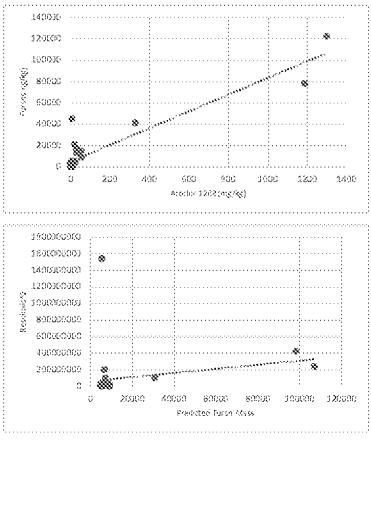
$H_0$  = homoscedasticity of residuals  
 $H_a$  = heteroscedasticity of residuals  
 $p < 0.05$

Status: Homoscedastic

ANOVA

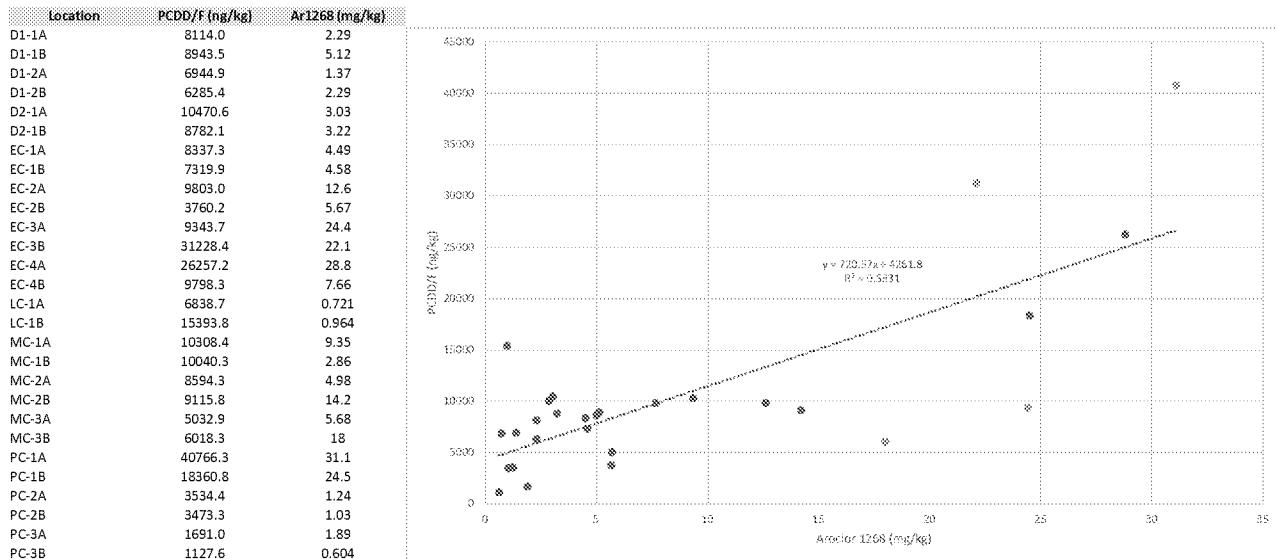
	df	SS	MS	F	Significance F
Regression	2	1.0918E+17	5.45898E+16	0.673304498	0.518085549
Residual	28	2.27017E+18	8.10774E+16		
Total	30	2.37935E+18			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	65107352.93	107523714.5	0.605516218	0.549713103	-155144991.8	285359697.7	-155144991.8	285359697.7
Pred PCDD/F (ng/kg)	2399.432246	15654.76226	1.053271714	0.879283284	-29667.89456	34466.75905	-29667.89456	34466.75905
Pred PCDD/F <sup>2</sup>	0.000636401	0.145350216	0.004378394	0.996537604	-0.29710002	0.298372821	-0.29710002	0.298372821



**APPENDIX C**  
**Cook's Distance Calculations for**  
**Co-location Cases 1-3**

**Case 1a: Co-Location of PCDD/F Concentration and Aroclor 1268 (Co-location Study Data)**



**Regression Analysis**

SUMMARY OUTPUT

	Mean	Std Dev (s)	Residual Std Dev ( $s_{e,adj}$ )
PCDD/F	10560	8853	
Ar1268	8.7	9.4	5824.8
DFFITS cutoff	0.69		
D <sub>i</sub> cutoff	0.14		
p (# parameters)	2		

ANOVA

	df	SS	MS	F	Significance F
Regression	1	1234007999	1234007999	36.37057423	2.27411E-06
Residual	26	882147413.2	33928746.66		
Total	27	2116155412			

Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%	
Intercept	4261.848447	1517.373234	2.80870148	0.009314981	1142.843096	7380.853798	1142.843096	7380.853798
Ar1268 (mg/kg)	720.5742178	119.4823181	6.030802122	2.27411E-06	474.9747954	966.1736401	474.9747954	966.1736401

Cooks Distance

Location	Ar1268 (mg/kg)	PCDD/F (ng/kg)	Residual ( $e_i$ )	Leverage ( $h_{ii}$ )	isr <sub>i</sub>	esr <sub>i</sub>	Cook's Dist (D <sub>i</sub> )	DFFITS
D1-1A	2.29	8114.0	2202.036594	0.053222839	0.388523003	0.382088925	0.0042428	0.0905919
D1-1B	5.12	8943.5	992.311558	0.041230224	0.173983064	0.170703829	0.0006509	0.0353992
D1-2A	1.37	6944.9	1695.864875	0.058573137	0.300064103	0.294747862	0.0028010	0.0735202
D1-2B	2.29	6285.4	373.4365943	0.053222839	0.065888418	0.064614304	0.0001220	0.0153198
D2-1A	3.03	10470.6	4025.411673	0.049436206	0.708819667	0.70186943	0.0130649	0.1600620
D2-1B	3.22	8782.1	2200.02572	0.048538312	0.387207381	0.380787572	0.0038243	0.0860061
EC-1A	4.49	8337.3	840.0733152	0.043167778	0.147451503	0.144648586	0.0004922	0.0307793
EC-1B	4.58	7319.9	-242.1783644	0.0429825	-0.042500601	-0.041676715	0.0000406	-0.0088341
EC-2A	12.6	9803.0	-3538.083591	0.041981381	-0.620579164	-0.613085463	0.0084381	-0.1283400
EC-2B	5.67	3760.2	-4587.304262	0.039681706	-0.803648312	-0.798015853	0.0133437	-0.1622180
EC-3A	24.2	9343.7	12300.15936	0.138891866	-2.31361211	2.544417982	0.33113132	1.6211277
EC-3B	23.1	31228.4	11030.86134	0.138891866	2.31361211	-2.544417982	-0.33113132	-1.6211277
EC-4A	28.8	26257.2	1242.814081	0.205020125	0.239300821	0.234912601	0.0073841	0.1192962
EC-4B	7.66	9798.3	16.85304485	0.036205683	0.00294715	0.002889919	0.0000002	0.0005601
LC-1A	0.721	6638.7	2057.317542	0.062775881	0.364834326	0.35866875	0.0044577	0.0928257
LC-1B	0.964	15393.8	2047.31801	0.061160768	1.849308615	1.945883672	0.1113962	0.4966583
MC-1A	9.35	10308.4	-690.8173832	0.035870504	-0.120784627	-0.118472314	0.0002714	-0.0228517
MC-1B	2.86	10040.3	3717.60929	0.050265336	0.654905581	0.647551035	0.0113499	0.1489729
MC-2A	4.98	8594.3	743.9919485	0.0416655038	0.130474506	0.127982685	0.0003701	0.0266857
MC-2B	14.2	9115.8	-5378.202339	0.048254842	-0.946439573	-0.944472356	0.0227078	-0.2126666
MC-3A	5.68	5032.9	-3321.810004	0.039655907	-0.581938976	-0.574391113	0.0065921	-0.1167208
MC-3B	18	6018.3	11213.28437	0.071785656	-1.3593246886	-2.129795656	0.1344102	0.3933900
PC-1A	31.1	49786.3	14094.88338	0.24671156	2.786734995	3.263131114	1.2673813	1.8643209
PC-1B	24.5	18360.8	-3555.116783	0.140213853	-0.658225558	-0.650889215	0.0353281	-0.2628496
PC-2A	1.24	3534.4	-1620.960477	0.059386592	-0.286934609	-0.281809074	0.0025990	-0.0708098
PC-2B	1.03	3473.3	-1530.739891	0.060730677	-0.271158	-0.266269059	0.0023770	-0.0677064
PC-3A	1.89	1691.0	-3932.733719	0.055461537	-0.694705615	-0.68762671	0.0141692	-0.1666245
PC-3B	0.604	1127.6	-3569.505275	0.06357125	-0.633266844	-0.6258143	0.0136122	-0.1630566

$$(1) e_i = f(x_i) - f(\bar{x})$$

$$(4) esr_i = isr_i \sqrt{\frac{n-p-1}{n-p-isr_i^2}}$$

$$(7) s_{e,adj} = \sqrt{\frac{(n-1)s_e^2}{(n-2)}}$$

$$(2) h_{ii} = \frac{1}{n} + \frac{1}{n-1} \left( \frac{x_i - \mu_x}{s_x} \right)^2$$

$$(5) D_i = \frac{isr_i^2}{p} \left( \frac{h_{ii}}{1-h_{ii}} \right)$$

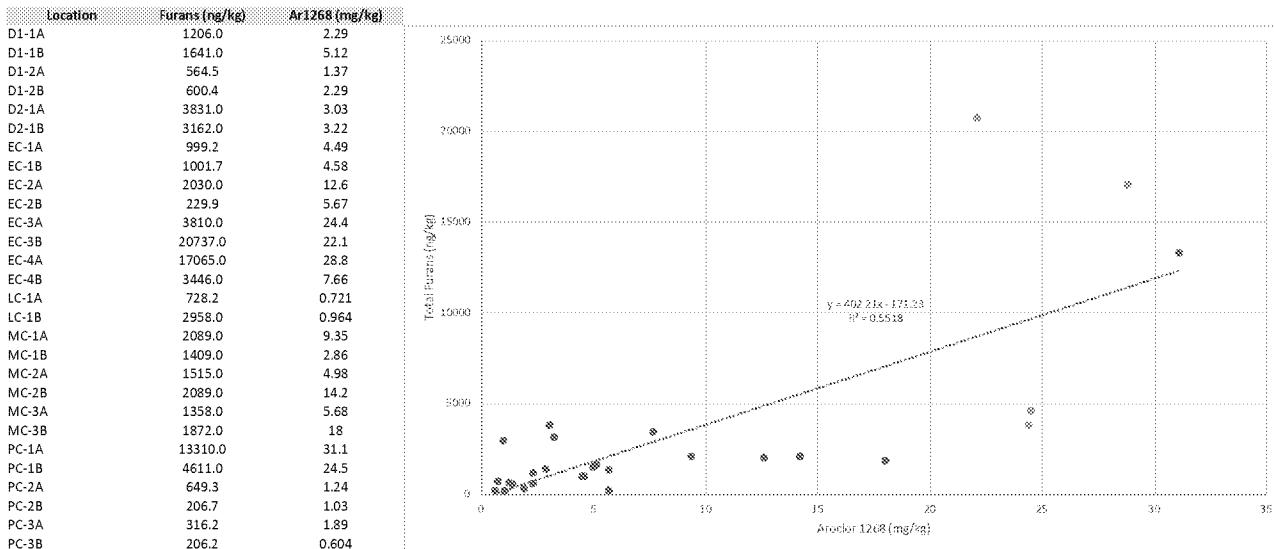
$$(8) DFFITS cutoff = 2 \sqrt{\frac{p+1}{n-p-1}}$$

$$(3) isr_i = \frac{e_i}{s_{e,adj} \sqrt{1-h_{ii}}}$$

$$(6) DFFITS_i = esr_i \sqrt{\frac{h_{ii}}{1-h_{ii}}}$$

$$(9) D_i cutoff = \frac{4}{n}$$

**Case 1b: Co-location of Furan Congener Concentration and Aroclor 1268 (Co-location Study Data)**



**Regression Analysis**

SUMMARY OUTPUT

Regression Statistics		Mean	Stnd Dev (s)	Residual Stnd Dev (s <sub>resid</sub> )
Multiple R	0.74280808	PCDD/F	3344	5080
R Square	0.551763843	Ar1268	8.7	9.4
Adjusted R Square	0.534523991	DFFITS cutoff	0.69	3465.9
Standard Error	3465.935399	D <sub>cutoff</sub>	0.14	
Observations	28	p (# parameters)	2	

ANOVA

	df	SS	MS	F	Significance F
Regression	1	384468380	384468380	32.00513772	5.98608E-06
Residual	26	312330413	12012708.19		
Total	27	696798793			

Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	-171.2333681	902.8777988	-0.189652873	0.851054	-2027.125263	-2027.125263	1684.658527
Ar1268 (mg/kg)	402.2073895	71.09518608	5.657308346	5.98608E-06	256.0691416	256.0691416	548.3456375

Cooks Distance

Location	Ar1268 (mg/kg)	Furans (mg/kg)	Residual (e <sub>i</sub> )	Leverage (h <sub>ii</sub> )	isr <sub>i</sub>	esr <sub>i</sub>	Cook's Dist (D <sub>i</sub> )	DFFITS <sub>i</sub>
D1-1A	2.29	1206.0	456.1784461	0.053222839	0.13526549	0.13268646	0.0005143	0.0314595
D1-1B	5.12	1641.0	-247.0684663	0.041230224	-0.072801393	-0.071394916	0.0001140	-0.0148053
D1-2A	1.37	564.5	184.7092444	0.058573137	0.054925608	0.053862115	0.0000938	0.0134351
D1-2B	2.29	600.4	-149.4215539	0.053222839	-0.044306648	-0.043447883	0.0000552	-0.0103013
D2-1A	3.03	3831.0	2783.544978	0.049436208	0.823734291	0.818488841	0.0176445	0.1866572
D2-1B	3.22	3162.0	2038.125574	0.048538312	0.602857713	0.595326109	0.0092703	0.1344626
EC-1A	4.49	999.2	-635.4778109	0.043316778	-0.18745449	-0.18393859	0.0007955	-0.0391396
EC-1B	4.58	1001.7	-669.176476	0.04299825	-0.197362136	-0.193674627	0.0008751	-0.0410527
EC-2A	12.6	2030.0	-2866.57974	0.04198131	-0.844999734	-0.840207823	0.0156446	-0.1758846
EC-2B	5.67	229.9	-1879.382531	0.039681706	-0.5533337	-0.545811612	0.0063259	-0.1109508
EC-3A	24.8	3810.0	-3833.626838	0.138893866	1.813448883	1.802873366	0.26532277	0.78414448
EC-3B	22.1	20137.0	-12013.45038	0.110089304	0.6777617803	0.2061113174	0.3427180	1.84341338
EC-3C	28.8	3162.0	-3632.66653	0.205011183	0.829111249	0.9213244883	0.4314387	0.91332288
EC-4B	7.66	3446.0	536.3247643	0.036205633	0.157621409	0.154634407	0.0004667	0.0299711
LC-1A	0.721	728.2	609.4418402	0.062775881	0.181631042	0.17821699	0.0011048	0.0461237
LC-1B	0.964	2958.0	2741.505445	0.061160768	0.816343679	0.810951217	0.0217069	0.2069834
MC-1A	9.35	2089.0	-1500.405724	0.035870505	-0.440880168	-0.433943692	0.0036159	-0.0837017
MC-1B	2.86	1409.0	429.920234	0.050265336	0.127281791	0.124848967	0.0004287	0.0287222
MC-2A	4.98	1515.0	-316.7594318	0.041665038	-0.093357761	-0.091560164	0.0001895	-0.0190912
MC-2B	14.2	2089.0	-3451.111563	0.048254842	-1.02065319	-1.021506155	0.0264087	-0.2300123
MC-3A	5.68	1358.0	-755.3046044	0.039655907	-0.222376164	-0.218265435	0.0010210	-0.0443533
MC-3B	18	1872.0	-5196.499643	0.071788374	-1.556205634	-1.602438766	0.0936510	-0.4456415
PC-1A	31.1	13310.0	972.5835536	0.246071156	0.32317762	0.317540161	0.0170444	0.1814111
PC-1B	24.8	3810.0	-3833.626838	0.138893866	0.829111249	0.9213244883	0.3427180	0.91332288
PC-2A	1.24	649.3	321.7962051	0.059386592	0.095731502	0.093889009	0.0002893	0.0235914
PC-2B	1.03	206.7	-36.34024312	0.067030677	-0.010818631	-0.010608564	0.0000038	-0.0026975
PC-3A	1.89	316.2	-272.7385981	0.055461537	-0.080968541	-0.079406199	0.0001925	-0.0192416
PC-3B	0.604	206.2	134.5001048	0.06357125	0.040101885	0.03932435	0.0000546	0.0102460

$$(1) e_i = f(x_i) - f(\bar{x})$$

$$(4) esr_i = isr_i \sqrt{\frac{n-p-1}{n-p-isr_i^2}}$$

$$(7) s_{e,adj} = \sqrt{\frac{(n-1)s_e^2}{(n-2)}}$$

$$(2) h_{ii} = \frac{1}{n} + \frac{1}{n-1} \left( \frac{x_i - \mu_x}{s_x} \right)^2$$

$$(5) D_i = \frac{isr_i^2}{p} \left( \frac{h_{ii}}{1-h_{ii}} \right)$$

$$(8) DFFITS cutoff = 2 \sqrt{\frac{p+1}{n-p-1}}$$

$$(3) isr_i = \frac{e_i}{s_{e,adj} \sqrt{1-h_{ii}}}$$

$$(6) DFFITS_i = esr_i \sqrt{\frac{h_{ii}}{1-h_{ii}}}$$

$$(9) D_i cutoff = \frac{4}{n}$$

**Case 2a: Co-location of PCDD/F Concentration and Aroclor 1268 (Cumulative Data Set)**

Location	PCDD/F (mg/kg)	Aroclor 1268 (mg/kg)
36	27038	55
61	141906	1300
68	64192	330
1718	18409	56
86048	2981	1.4
C-1S	10834	0.099
C-6	59189	7.58
C-8	10654	2.2
111	9396	6.1
EPA-E3	240328	3800
EPA-F2	94058	1188
EPA-H1	538204	4000
GRID MARSH	5980	6.1
117	2133	11
110	3049	0.25
100	856	1.1
101	2058	0.085
102	2678	0.13
D1-1A	8114	2.29
D1-1B	8944	5.12
D1-2A	6945	1.37
D1-2B	6285	2.29
D2-1A	10471	3.03
D2-1B	8782	3.22
EC-1A	8337	4.49
EC-1B	7320	4.58
EC-2A	9803	12.6
EC-2B	3760	5.67
EC-3A	9344	24.4
EC-3B	31228	22.1
EC-4A	26257	28.8
EC-4B	9798	7.66
LC-1A	6839	0.721
LC-1B	15394	0.964
MC-1A	10308	9.35
MC-1B	10040	2.86
MC-2A	8594	4.98
MC-2B	9116	14.2
MC-3A	5033	5.68
MC-3B	6018	18
PC-1A	40766	31.1
PC-1B	18361	24.5
PC-2A	3534	1.24
PC-2B	3473	1.03
PC-3A	1691	1.89
PC-3B	1128	0.604

**Regression Analysis**

**SUMMARY OUTPUT**

Regression Statistics	Mean	Stnd Dev (s)	Residual Stnd Dev (s <sub>res</sub> )
Multiple R	0.93149109		
R Square	0.86767565		
Adjusted R Square	0.864668279		
Standard Error	31970.40714		
Observations	46		
	DFFITS cutoff	0.53	
	D <sub>i</sub> cutoff	0.09	
	p (# parameters)	2	

**ANOVA**

	df	SS	MS	F	Significance F
Regression	1	2.94894E+11	2.94894E+11	288.5162765	6.07035E-21
Residual	44	49972705045	1022106933		
Total	45	3.39867E+11			

**Coefficients**

Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%	
Intercept	9519.33582	4909.876566	2.020282116	0.049467713	24.12979434	19814.54185	24.12979434	19814.54185
Aroclor 1268 (mg/kg)	97.4922222	5.739642072	16.98576688	6.07035E-21	85.92473368	109.0597107	85.92473368	109.0597107

**Cook's Distance**

Location	Aroclor 1268 (mg/kg)	PCDD/F (mg/kg)	Residual (s <sub>res</sub> )	Leverage (h <sub>ii</sub> )	tstat	sstat	Cook's Dist (D)	DFFITS
36	55	27038	11756.4918	0.022834415	0.367845611	0.364201958	0.0015810	0.0576741
61	1300	141906	5246.77403	0.05799874	0.16720087	0.165342475	0.0008600	0.0410268
68	330	64192	22100.22988	0.022004026	0.691194338	0.687034788	0.0053745	0.1030531
1718	56	18409	3030.299858	0.02282564	0.094813637	0.0937939593	0.0001050	0.0143258
86048	1.4	2981	-7074.824924	0.023563944	-0.221444913	-0.219363123	0.0005917	-0.0340265
C-1S	0.099	10834	905.014068	0.023551696	0.02837549	0.0280405	0.0000097	0.0043522
C-6	7.58	59189	48530.67228	0.023470389	1.515897118	1.542585945	0.0277266	0.2391480
C-8	2.2	10654	520.5814229	0.023551696	0.016294309	0.016108131	0.0000032	0.0025017
111	6.1	9396	-1117.671376	0.023492571	0.034972393	0.034582963	0.0000147	-0.0053640
EC-1A	8337	94088	16552.39579	0.050745383	-1.034817139	-1.034930153	0.0269872	-0.13323501
EC-1B	4.49	8782	-16552.39579	0.050745383	-1.034817139	-1.034930153	0.0269872	-0.13323501
EC-2A	8337	94088	16552.39579	0.050745383	-1.034817139	-1.034930153	0.0269872	-0.13323501
EC-2B	4.49	8782	-16552.39579	0.050745383	-1.034817139	-1.034930153	0.0269872	-0.13323501
EC-3A	28.8	26257	-4534.038487	0.023492571	-0.141912072	-0.1403232203	0.0002422	-0.0217640
EC-3B	7.66	9798	-867.8262422	0.023469194	-0.071619198	-0.071685179	0.0000898	-0.0041627
LC-1A	0.721	6839	-3150.927712	0.023574376	-0.095371122	-0.094257255	0.001094	-0.0146271
LC-1B	0.964	15394	-3045.951908	0.023551499	-0.095337122	-0.0941607053	0.0002122	-0.0064399
MC-1A	9.35	10308	-522.4880977	0.023444061	-0.063495348	-0.062772539	0.0000485	-0.0097486
MC-1B	2.86	10040	-157.8635757	0.023541623	-0.0049411138	-0.004884667	0.0000003	-0.007584
MC-2A	4.98	8594	-1810.547087	0.023509455	-0.092459457	-0.091411642	0.0001016	-0.0140966
MC-2B	14.2	9116	-2187.925375	0.023260257	-0.0594950033	-0.05950337	0.0042787	0.0918247
MC-3A	5.68	5033	-5440.191642	0.023349881	-0.170247551	-0.1683823979	0.0003498	-0.0261209
MC-3B	18	6018	-5655.89582	0.023319215	-0.17700958	-0.175498884	0.0003740	-0.0270477
PC-1A	31.1	40766	27814.95607	0.023136832	0.8710429147	0.867985456	0.0089724	0.1335820
PC-1B	24.5	18361	6052.954736	0.0232126833	0.189425697	0.1873317163	0.0042666	0.0288983
PC-2A	1.24	3534	-6505.826176	0.023566403	-0.203657526	-0.201402866	0.0005004	-0.0312889
PC-2B	1.03	3473	-6546.452809	0.023569698	-0.204907246	-0.20266919	0.0005868	-0.03144868
PC-3A	1.89	1691	-8412.59612	0.023355644	-0.03116868	-0.026014594	0.0008364	-0.0406632
PC-3B	0.604	1128	-8850.651122	0.023576178	-0.277030734	-0.274103719	0.0009265	-0.0425924

$$(1) \hat{e}_i = f(\mathbf{x}_i) - f(\mathbf{\bar{x}})$$

$$(4) esr_i = i s_{\bar{x}} \sqrt{\frac{1-p}{n-p}}$$

$$(7) s_{\bar{x},adj} = \sqrt{\frac{(n-1)s_{\bar{x}}^2}{(n-2)}}$$

$$(2) h_{ii} = \frac{1}{n} + \frac{1}{n-1} \left( \frac{x_i - \bar{x}_i}{s_x} \right)^2$$

$$(5) D_i = \frac{i s_{\bar{x}}^2}{p} \left( \frac{h_{ii}}{1-h_{ii}} \right)$$

$$(8) DFFITS cutoff = 2 \sqrt{\frac{p+1}{n-p-1}}$$

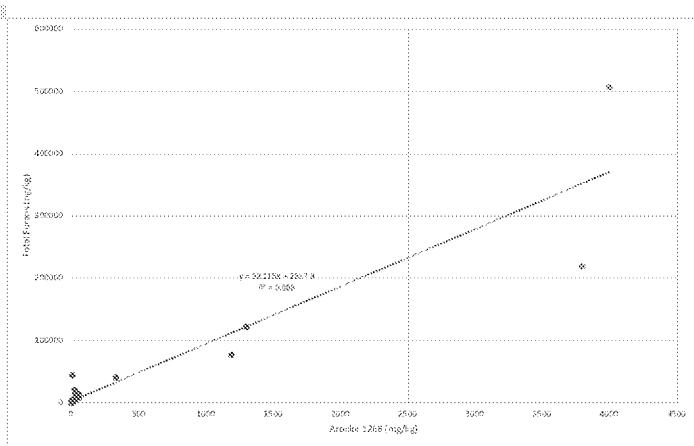
$$(3) isr_i = \frac{s_{\bar{x}}}{s_{\bar{x},adj} \sqrt{1-h_{ii}}}$$

$$(6) DFFITS_i = esr_i \sqrt{\frac{h_{ii}}{1-h_{ii}}}$$

$$(9) D_i cutoff = \frac{4}{n}$$

**Case 2b: Co-location of Furan Congener Concentration and Aroclor 1268 (Cumulative Data Set)**

Location	Furan (mg/kg)	Aroclor 1268 (mg/kg)
36	14468	55
61	122400	1300
68	40850	330
1718	8750	56
BR048	391	1.4
C-15	1348	0.1
C-6	44710	8
C-8	2826	2
111	5036	6
EPA-E3	219200	3800
EPA-F2	77700	1188
EPA-H1	507600	4000
GRIB MARSH	3690	6
117	148	11.0
110	630	0.25
100	71	1.1
101	161	0.1
102	147	0.1
D1-1A	1206	2.3
D1-1B	1641	5.1
D1-2A	565	1.4
D1-2B	600	2.3
D2-1A	3831	3.0
D2-1B	3162	3
EC-1A	999	4.5
EC-1B	1002	4.6
EC-2A	2030	12.6
EC-2B	230	5.7
EC-3A	3810	24.4
EC-3B	20737	22
EC-4A	17065	29
EC-4B	3446	8
LC-1A	728	1
LC-1B	2958	1.0
MC-1A	2089	9
MC-1B	1409	2.9
MC-2A	1515	5.0
MC-2B	2089	14.2
MC-3A	1358	5.7
MC-3B	1872	18.0
PC-1A	13310	31.1
PC-1B	4611	25
PC-2A	649	1
PC-2B	207	1.0
PC-3A	316	1.9
PC-3B	206	0.6



**Regression Analysis**  
SUMMARY OUTPUT

	Mean	Stnd Dev (s)	Residual Stnd Dev (Sres)
PCDD/F	24864	82097	
Aroclor 1268	239.3	830.3	30505.5
DFITTS cutoff	0.53		
Standard Error	0.09	D. cut off	
Observations	46	p (# parameters)	2

ANOVA

	df	SS	MS	F	Significance F
Regression	1	2.83263E+11	2.63263E+11	289.3310295	5.75115E-21
Residual	44	4003574067	90903956.1		
Total	45	3.03299E+11			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	2817.328495	4632.550728	0.608159232	0.546208528	-6518.96403	12153.62102	-6518.96403	12153.62102
Aroclor 1268 (mg/kg)	92.1153293	5.415448373	17.00973338	5.75115E-21	81.20121388	103.029452	81.20121388	103.029452

Cook's Distance

Location	Aroclor 1268 (mg/kg)	Furan (mg/kg)	Residual (s)	Leverage (h <sub>ii</sub> )	Infl.	err.	Cook's Dist (D <sub>i</sub> )	DFITTS
36	55	14468	6584.28115	0.022834415	0.218348236	0.215963784	0.0005570	0.0330144
61	1300	122400	-167.264791	0.05799874	-0.005649308	-0.00584742	0.0000010	-0.001385
68	330	40850	7634.10696	0.022004026	0.253070002	0.250359951	0.0007205	0.0375532
1718	56	8750	774.2128979	0.02282564	0.025674145	0.025380907	0.0000077	0.0038788
BR048	1.4	391	-2555.28995	0.023563948	-0.084769689	-0.083077075	0.0000867	-0.0130193
C-15	0.1	1348	-1478.447908	0.023583958	-0.049468623	-0.048487595	0.0000291	-0.0075357
C-6	8	44710	41194.43686	0.023470389	1.366526842	1.380521713	0.024409	0.2140231
C-8	2	2826	-193.9822459	0.02355169	-0.006435165	-0.00636162	0.0000005	-0.0009889
111	8	5036	1656.848974	0.023492571	0.054962623	0.054336324	0.0000563	0.0084279
EPA-E3	1188	77700	-2817.328495	0.023492571	-0.087922309	-0.087025833	0.0000752	-0.0121212
EPA-F2	1188	77700	-34550.34402	0.050745383	-1.162752697	-1.167352697	0.0361102	-0.1698807
EC-1A	4.5	999	-2231.72634	0.023563948	-0.094485486	-0.093415094	0.0001077	-0.0145132
EC-1B	4.6	1002	-2237.51672	0.023585553	-0.094485486	-0.093415094	0.0001077	-0.0145132
EC-2A	12.6	2030	-1947.98169	0.023396203	-0.064617176	-0.0638817	0.0000500	-0.0098876
EC-2B	5.7	230	-3109.722433	0.023499042	-0.103159112	-0.101992446	0.0001280	-0.0152818
EC-3A	24.4	3810	-1279.626501	0.023398218	-0.041624557	-0.041149642	0.0000206	-0.0063457
EC-3B	22	20737	15883.92625	0.023262527	0.526854433	0.522483703	0.0033051	0.0806282
EC-4A	29	17065	11594.74992	0.023167877	0.384568514	0.380913836	0.0017538	0.0586470
EC-4B	8	3446	-76.93194539	0.023469194	-0.005252032	-0.002522885	0.0000001	-0.0030391
LC-1A	1	728	-2155.54365	0.023574378	-0.070588088	-0.070695646	0.0000617	-0.0109848
LC-1B	1.0	2958	51.8732393	0.023579642	0.001720289	0.00170161	0.0000000	0.002643
MC-1A	9	2089	-1589.606858	0.023444046	-0.052730691	-0.052129682	0.0000334	-0.0080771
MC-1B	2.9	1409	-1671.78347	0.023541623	-0.05549268	-0.054827343	0.0000371	-0.0085131
MC-2A	5.0	1515	-1761.652853	0.0235945	-0.058420213	-0.057754772	0.0000411	-0.0089614
MC-2B	14.2	2089	-2036.366223	0.023372893	-0.065748204	-0.065779661	0.0000546	-0.0103302
MC-3A	5.7	1358	-1982.45588	0.02349881	-0.065767079	-0.065018645	0.0000520	-0.010861
MC-3B	18.0	1872	-2603.04488	0.023318215	-0.086354984	-0.085375273	0.0000990	-0.0131918
PC-1A	31.1	13310	7627.84651	0.023136832	0.25993611	0.250284268	0.0007580	0.0385184
PC-1B	25	4611	-463.154152	0.023226833	-0.01536115	-0.015186583	0.0000218	-0.0023418
PC-2A	1	649	-2282.251508	0.023356403	-0.07511953	-0.074851521	0.0000692	-0.0163286
PC-2B	1.0	207	-2705.507288	0.023356028	-0.089753289	-0.089735627	0.0000973	-0.0137865
PC-3A	1.9	316	-2675.26474	0.0235564	-0.088748145	-0.087741701	0.0000950	-0.0136282
PC-3B	0.6	206	-2666.766156	0.023576178	-0.086468376	-0.087465055	0.0000945	-0.0135910

$$(1) \quad e_i = f(x_i) - f(\bar{x})$$

$$(4) \quad esr_i = i\sigma_{\bar{r}} \sqrt{\frac{n-p-1}{n-p-i\sigma_{\bar{r}}^2}}$$

$$(7) \quad s_{e,adj} = \sqrt{\frac{(n-1)s_e^2}{(n-2)}}$$

$$(2) \quad h_{ii} = \frac{1}{n} + \frac{1}{n-1} \left( \frac{x_i - \bar{x}_x}{s_x} \right)^2$$

$$(5) \quad D_i = \frac{i\sigma^2}{p} \left( \frac{h_{ii}}{1-h_{ii}} \right)$$

$$(8) \quad DFFITS_{ci} = 2 \sqrt{\frac{p+1}{n-p-1}}$$

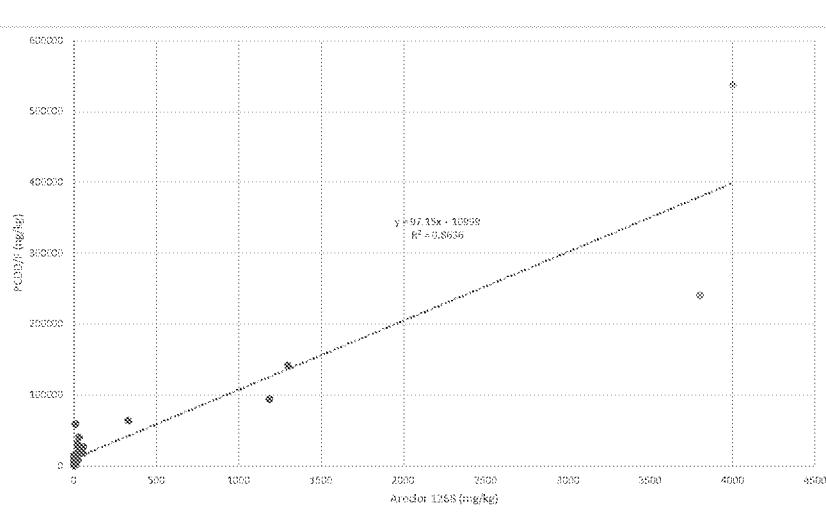
$$(3) \quad i\sigma_{\bar{r}} = \frac{s_i}{s_{\bar{r},adj} \sqrt{1-h_{ii}}}$$

$$(6) \quad DFFITS_{ci} = esr_i \sqrt{\frac{h_{ii}}{1-h_{ii}}}$$

$$(9) \quad D_i, cutoff = \frac{4}{n}$$

**Case 3a: Co-location of PCDD/F Concentration and Aroclor 1268 (Original Distribution)**

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)
36	27038	55
61	141906	1300
68	64192	330
1718	18409	56
BR048	2981	1.4
C-15	10834	0.099
C-6	59189	7.58
111	9396	6.1
EPA-E3	240328	3800
EPA-F2	94088	1188
EPA-H1	538204	4000
GRID MARSH	5980	6.1
117	2133	11
110	3049	0.25
100	856	1.1
101	2058	0.085
102	2678	0.13
D2-1A	10471	3.03
D2-1B	8782	3.22
EC-3A	9344	24.4
EC-3B	31228	22.1
EC-4A	26257	28.8
EC-4B	9798	7.66
LC-1A	6839	0.721
LC-1B	15394	0.964
PC-1A	40766	31.1
PC-1B	18361	24.5
PC-2A	3534	1.24
PC-2B	3473	1.03
PC-3A	1691	1.89
PC-3B	1128	0.604
D1-2A	6945	1.37
D1-2B	6285	2.29



Regression Analysis  
SUMMARY OUTPUT

Regression Statistics	PCDD/F	Mean	Std Dev (s)	Residual Std Dev (s <sub>res</sub> )
Multiple R	0.929288027	43140	101304	
R Square	0.863576236	330.8	969.0	38016.0
Adjusted R Square	0.85917547			
Standard Error	38015.98318	DFFITS cutoff	0.63	
Observations	33	D <sub>i</sub> cutoff	0.12	
		p (# parameters)	2	

ANOVA

	df	SS	MS	F	Significance F
Regression	1	2.83599E+11	2.83599E+11	196.2331389	5.93398E-15
Residual	31	44801664291	1445214977		
Total	32	3.28401E+11			

Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%	
Intercept	10998.59331	7004.20235	1.570284918	0.126501041	-3286.571562	25283.75818	-3286.571562	25283.75818
Ar1268 (mg/kg)	97.15010107	6.935169523	14.00832391	5.93398E-15	83.00572958	111.2944726	83.00572958	111.2944726

Cooks Distance

Location	Ar1268 (mg/kg)	PCDD/F (ng/kg)	Residual (e <sub>i</sub> )	Leverage (h <sub>ii</sub> )	Isr <sub>i</sub>	ex <sub>i</sub>	Cook's Dist (D <sub>i</sub> )	DFFITS <sub>i</sub>
36	55	27038	10696.05097	0.032835244	0.286092851	0.281812905	0.0013894	0.0519255
61	1300	141906	4612.274004	0.061561773	0.125240856	0.123235465	0.0005145	0.0315637
68	330	64192	21133.87236	0.030303054	0.056450157	0.0558237012	0.0049798	0.0986833
1718	56	18409	1970.201151	0.032816917	0.052697498	0.051842893	0.0000471	0.0095496
BR048	1.4	2981	-8135.603446	0.033914948	-0.218210517	-0.214827192	0.0008358	-0.0402510
C-15	0.099	10834	-174.2112141	0.033943532	-0.00466239	-0.004586576	0.0000004	-0.0008597
C-6	7.58	59189	4754.00807	0.033780707	1.269897945	1.283066503	0.0281904	0.2399085
111	6.1	9396	-2194.841928	0.033312623	-0.058736267	-0.057784358	0.0000604	-0.0108098
LC-1A	0.721	6839	-4229.938534	0.033929852	-0.1132045	-0.1138663	0.0002250	-0.0208747
LC-1B	0.964	15394	4301.553992	0.033924514	0.115120753	0.112327961	0.0002327	0.0212265
PC-1A	31.1	40766	26746.33855	0.033293056	0.715567639	0.709818174	0.0088172	0.1317275
PC-1B	24.5	18361	4982.029213	0.03342618	0.133297661	0.131167671	0.0003072	0.0243923
PC-2A	1.24	3534	-7584.659436	0.033918457	-0.20284542	-0.198816594	0.0007233	-0.0374406
PC-2B	1.03	3473	-7625.537915	0.033923065	-0.204074222	-0.200890707	0.0007312	-0.0376445
PC-3A	1.89	1691	-9491.207002	0.033904211	-0.254006672	-0.250136643	0.0011321	-0.0468591
PC-3B	0.604	1128	-9929.701972	0.033932423	-0.265745693	-0.26172626	0.0012403	-0.0490507
D1-2A	1.37	6945	-4186.78895	0.033915606	-0.112048826	-0.1102491	0.0002204	-0.0206570
D1-2B	2.29	6285	-4935.667042	0.033895459	-0.132089278	-0.129977924	0.0003061	-0.0243460

$$(1) e_i = f(\mathbf{x}_i) - f(\bar{\mathbf{x}})$$

$$(4) esr_i = isr_i \sqrt{\frac{n-p-1}{n-p-isr_i^2}}$$

$$(7) s_{e,adj} = \sqrt{\frac{(n-1)s_e^2}{(n-2)}}$$

$$(2) h_{ii} = \frac{1}{n} + \frac{1}{n-1} \left( \frac{x_i - \mu_x}{s_x} \right)^2$$

$$(5) D_i = \frac{isr_i^2}{p} \left( \frac{h_{ii}}{1-h_{ii}} \right)$$

$$(8) DFFITS cutoff = 2 \sqrt{\frac{p+1}{n-p-1}}$$

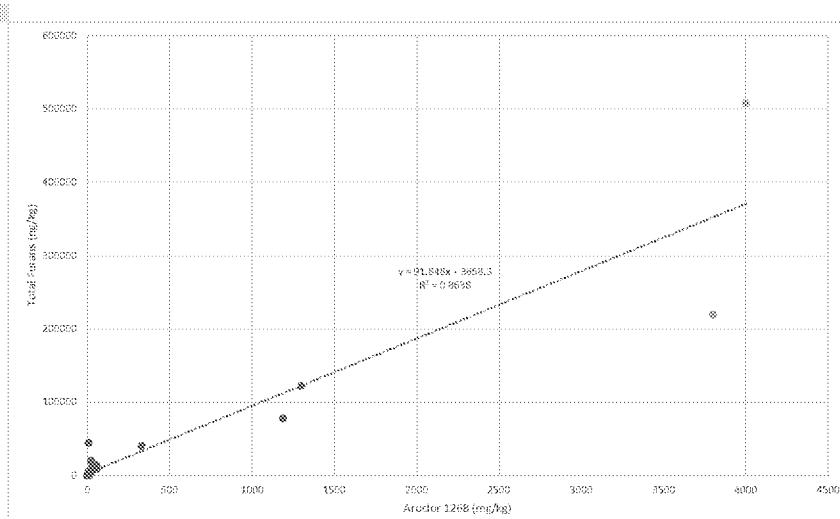
$$(3) isr_i = \frac{e_i}{s_{e,adj} \sqrt{1-h_{ii}}}$$

$$(6) DFFITS_i = esr_i \sqrt{\frac{h_{ii}}{1-h_{ii}}}$$

$$(9) D_i cutoff = \frac{4}{n}$$

**Case 3b: Co-location of Furan Mass and Aroclor 1268 (Original Distribution)**

Location	Furans (ng/kg)	Ar1268 (mg/kg)
36	14468	55
61	122400	1300
68	40850	330
1718	8750	56
BR048	391	1.4
C-15	1348	0.1
C-6	44710	8
111	5036	6
EPA-E3	219200	3800
EPA-F2	77700	1188
EPA-H1	507600	4000
GRID MARSH	3690	6
117	148	11.0
110	630	0.25
100	71	1.1
101	161	0.1
102	147	0.1
D2-1A	3831	3.0
D2-1B	3162	3
EC-3A	3810	24.4
EC-3B	20737	22
EC-4A	17065	29
EC-4B	3446	8
LC-1A	728	1
LC-1B	2958	1.0
PC-1A	13310	31.1
PC-1B	4611	25
PC-2A	649	1
PC-2B	207	1.0
PC-3A	316	1.9
PC-3B	206	0.6
D1-2A	565	1.37
D1-2B	600	2.29



Regression Analysis  
SUMMARY OUTPUT

Regression Statistics	PCDD/F	Mean	Stnd Dev (s)	Residual Stnd Dev (s <sub>adj</sub> )
Multiple R	0.929419365	34045	95762	
R Square	0.863820356	330.8	969.0	35904.1
Adjusted R Square	0.859427465			
Standard Error	35904.05431	DFFITS cutoff	0.63	
Observations	33	D <sub>i</sub> cutoff	0.12	
		p (# parameters)	2	

ANOVA

	df	SS	MS	F	Significance F
Regression	1	2.53489E+11	2.53489E+11	196.6404842	5.77075E-15
Residual	31	39962134596	1289101116		
Total	32	2.93452E+11			

Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%	
Intercept	3658.299321	6615.09293	0.553023118	0.58421401	-9833.27166	17149.8703	-9833.27166	17149.8703
Ar1268 (mg/kg)	91.84823482	6.549895133	14.02285578	5.77075E-15	78.48963563	105.206834	78.48963563	105.206834

Cook's Distance

Location	Ar1268 (mg/kg)	Furans (ng/kg)	Residual (e <sub>i</sub> )	Leverage (h <sub>ii</sub> )	isr <sub>i</sub>	esr <sub>i</sub>	Cook's Dist. (D <sub>i</sub> )	DFFITS <sub>i</sub>
36	55	14468	5758.047685	0.032835244	0.163072802	0.160489886	0.0004514	0.0295711
61	1300	122400	-661.0057633	0.061561773	-0.019004608	-0.018695678	0.0000118	-0.0047884
68	330	40850	6881.782246	0.030303054	0.194643283	0.191595253	0.0005920	0.0338696
1718	56	8750	-3395.886848	0.032816917	-0.001467018	-0.001443163	0.0000000	-0.0002658
BR048	1.4	391	-3395.886848	0.033914948	-0.096228128	-0.094677748	0.0001625	-0.0177392
C-15	0.1	1348	-2319.392291	0.033943532	-0.065724828	-0.064660566	0.0000759	-0.0121204
C-6	8	44710	40355.49064	0.033780707	1.143460816	1.149366543	0.0228563	0.2149092
111	6	5036	817.507447	0.033812623	0.023164213	0.022787731	0.0000094	0.0042629
117	11.0	148	-2319.392291	0.033812623	-0.014977228	-0.014733729	0.0000039	-0.0027563
EPA-F2	1188	77700	-35074.00229	0.054754456	-1.004776605	-1.004937006	0.0292404	-0.2418668
EPA-H1	31.1	13310	337650.37818	0.4793433777	5.3703856433	13.711616337	13.71223303	13.71223303
GRID MARSH	6	3690	-528.573628	0.033812623	-0.014977228	-0.014733729	0.0000039	-0.0027563
117	11.0	148	-4521.021904	0.03370751	-0.128096958	-0.126047306	0.0002862	-0.0235420
110	0.25	630	-3051.261379	0.033940208	-0.08646372	-0.08506797	0.0001313	-0.0159449
100	1.1	71	-3688.832379	0.033921529	-0.104529585	-0.102847931	0.0001918	-0.0192720
101	0.1	161	-3505.007421	0.03394384	-0.099321727	-0.097722182	0.0001733	-0.0183178
102	0.1	147	-3522.887591	0.033942849	-0.099822834	-0.0988220804	0.0001751	-0.0184110
D2-1A	3.0	3831	-105.5994721	0.033879294	-0.02992282	-0.022943624	0.0000002	-0.0005512
D2-1B	3	3162	-792.0506367	0.03387515	-0.022443616	-0.02078834	0.0000088	-0.0041343
EC-3A	24.4	3810	-2089.39625	0.033428219	-0.059191625	-0.058232386	0.0000606	-0.0108294
EC-3B	22	20737	15048.85469	0.033475308	0.426337447	0.420639658	0.0031477	0.0782827
EC-4A	29	17065	10761.47152	0.033339118	0.304853437	0.300346687	0.0016026	0.0557780
EC-4B	8	3446	-915.8567993	0.033778985	-0.025950507	-0.025528796	0.0000118	-0.0047733
LC-1A	1	728	-2996.321898	0.033929852	-0.084906443	-0.083535472	0.0001266	-0.0156552
LC-1B	1.0	2958	-788.3410189	0.033924514	-0.022353239	-0.021989925	0.0000088	-0.0041207
PC-1A	31.1	13310	6795.220576	0.033293056	0.192491983	0.189475094	0.0006380	0.0351626
PC-1B	25	4611	-1297.581074	0.03342618	-0.03675983	-0.036162858	0.0000234	-0.0067249
PC-2A	1	649	-3122.891132	0.033918457	-0.088492499	-0.087064498	0.0001375	-0.0163137
PC-2B	1.0	207	-3546.203002	0.033923065	-0.10048801	-0.098870053	0.0001773	-0.0185271
PC-3A	1.9	316	-3515.692484	0.033904211	-0.099622467	-0.098018173	0.0001741	-0.0183621
PC-3B	0.6	206	-3507.575654	0.033932423	-0.099393916	-0.097793231	0.0001735	-0.0183279
D1-2A	1.37	565	-3219.631402	0.033915606	-0.091233667	-0.089762145	0.0001461	-0.0168184
D1-2B	2.29	600	-3268.231778	0.033895459	-0.092609874	-0.091116527	0.0001505	-0.0170669

$$(1) e_i = f(x_i) - f(\bar{x})$$

$$(4) esr_i = isr_i \sqrt{\frac{n-p-1}{n-p-isr_i^2}}$$

$$(7) s_{e,adj} = \sqrt{\frac{(n-1)s_e^2}{(n-2)}}$$

$$(2) h_{ii} = \frac{1}{n} + \frac{1}{n-1} \left( \frac{x_i - \bar{x}}{s_x} \right)^2$$

$$(5) D_i = \frac{isr_i^2}{p} \left( \frac{h_{ii}}{1-h_{ii}} \right)$$

$$(8) DFFITS cutoff = 2 \sqrt{\frac{p+1}{n-p-1}}$$

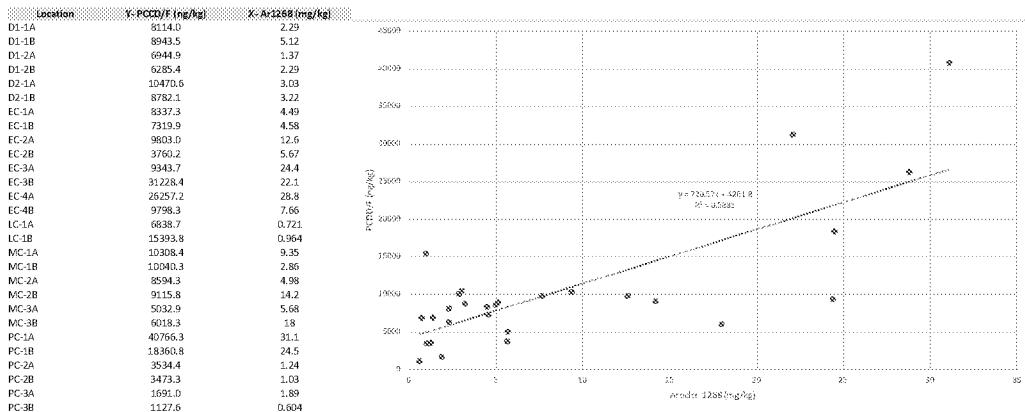
$$(3) isr_i = \frac{e_i}{s_{e,adj} \sqrt{1-h_{ii}}}$$

$$(6) DFFITS_i = esr_i \sqrt{\frac{h_{ii}}{1-h_{ii}}}$$

$$(9) D_i cutoff = \frac{4}{n}$$

**APPENDIX D**  
**Calculations for Co-location Cases 1-3**

**Case 1a: Co-location of PCDD/F Concentration and Aroclor 1268 (Co-location Study Data)**



**Regression Analysis**

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.763633914
R Square	0.583136754
Adjusted R Square	0.567103553
Standard Error	5824.838767
Observations	28

$H_0$  = PCDD/F not correlated to Aroclor 1268  
 $H_A$  = PCDD/F correlated to Aroclor 1268  
 $p < 0.05$   
**Status: PCDD/F correlated to Aroclor 1268**

ANOVA

	df	ss	ms	f	Significance F
Regression	1	1234007999	1234007999	36.37057423	2.27411E-06
Residual	26	882147413.2	33928746.66		
Total	27	2116155412			

Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%	
Intercept	4261.848447	1517.373234	2.80870148	0.009334981	1142.843096	7380.853798	1142.843096	7380.853798
Ar1268 (mg/kg)	720.5742178	119.4523181	6.030802122	2.27411E-06	474.9747954	966.1736401	474.9747954	966.1736401

Pearson Correlation Analysis

Location	Log X	Log Y	(Log X)^2	Log Y^2	LOG X * LOG Y
D1-1A	0.4	3.8	0.124981574	15.28221831	-1.496681463
D1-1B	0.7	4.0	0.502053878	15.61441161	-2.02605578
D1-2A	0.1	3.8	0.016932513	14.75389763	0.525234754
D1-2B	0.4	3.8	0.124981574	14.4733298	1.366774959
D2-1A	0.5	4.0	0.231787005	16.16037141	1.935385679
D2-1B	0.5	3.9	0.257917586	15.55196817	2.002779592
EC-1A	0.7	3.9	0.425425289	15.57440401	2.557474489
EC-1B	0.7	3.9	0.43674318	14.93440094	2.553918342
EC-2A	1.1	4.0	1.210915337	15.53094669	4.391973881
EC-2B	0.8	3.6	0.567887427	12.7821333	2.69421384
EC-3A	1.4	4.0	1.92485053	15.70502022	5.508657508
EC-3B	1.3	4.5	1.807390586	20.20097731	6.042437395
EC-4A	1.5	4.4	2.129826433	19.52975653	6.449417934
EC-4B	0.9	4.0	0.7831860517	15.92928417	3.529093031
LC-1A	-0.1	3.8	0.020182389	14.70702215	-0.544814503
LC-1B	0.0	4.2	0.00253541	17.53386518	0.0666741966
MC-1A	1.0	4.0	0.942475184	16.10570411	3.896052574
MC-1B	0.5	4.0	0.208269956	16.01397657	1.8262161262
MC-2A	0.7	3.9	0.486128756	15.47801233	2.743047008
MC-2B	1.2	4.0	1.327765429	15.67997476	4.562825381
MC-3A	0.8	3.7	0.569041412	13.70345874	2.792460475
MC-3B	1.3	3.8	1.575709062	14.28442245	4.744269586
PC-1A	1.5	4.6	2.228333579	21.25487804	6.8832075256
PC-1B	1.4	4.3	1.92978241	18.18077158	5.923253599
PC-2A	0.1	3.5	0.008727611	12.59054543	0.331849632
PC-2B	0.0	3.5	0.0016479	12.53685601	0.045453304
PC-3A	0.3	3.2	0.076431129	10.42091115	0.892458406
PC-3B	-0.2	3.1	0.04794482	9.315580021	-0.668306687

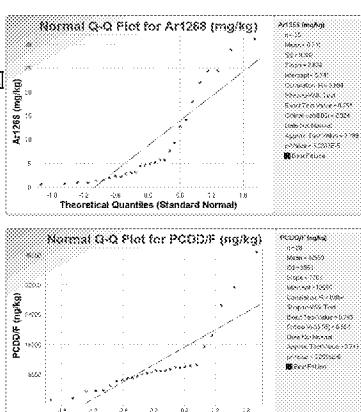
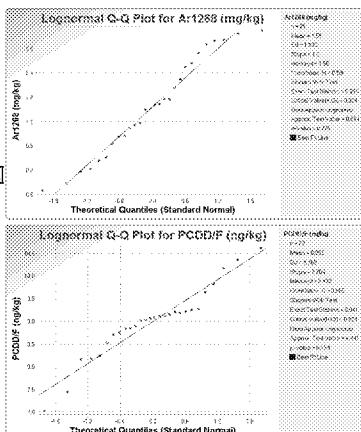
Spearman Correlation Analysis

Location	PCDD/F Rank	Ar1268 Rank	Rank Difference	Difference^2
D1-1A	17	20.5	-3.5	12.25
D1-1B	13	13	0	0
D1-2A	19	23	-4	16
D1-2B	21	20.5	0.5	0.25
D2-1A	6	18	-12	144
D2-1B	14	17	3	9
EC-1A	16	15	0	0
EC-1B	18	15	3	9
EC-2A	9	8	1	1
EC-2B	24	12	12	144
EC-3A	11	4	7	49
EC-3B	2	5	-3	9
EC-4A	3	2	1	1
EC-4B	10	10	0	0
LC-1A	20	27	-7	49
LC-1B	5	26	-21	441
MC-1A	7	9	-2	4
MC-1B	8	19	-11	121
MC-2A	15	14	1	1
MC-2B	12	7	5	25
MC-3A	23	11	12	144
MC-3B	22	6	16	256
PC-1A	1	1	0	0
PC-1B	4	3	1	1
PC-2A	25	24	1	1
PC-2B	26	25	1	1
PC-3A	27	22	5	25
PC-3B	28	28	0	0

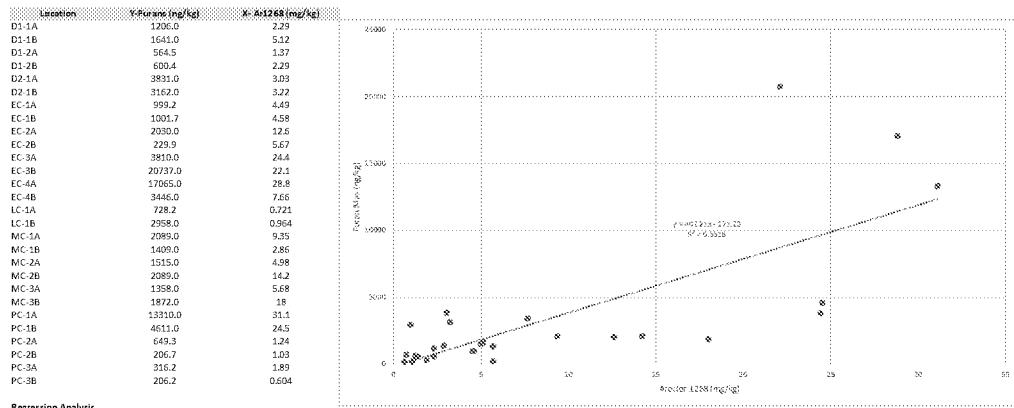
$$t_s = 1 - \frac{6 \sum d_i^2}{n(n^2 - 1)}$$

$$n = 28$$

$$t_s = 0.599$$



**Case 1b: Co-location of Furan Congener Concentration and Arodror 1268 (Co-location Study Data)**



**Regression Analysis**

**SUMMARY OUTPUT**

Regression Statistics	
Multiple R	0.74280808
R Square	0.551763843
Adjusted R Square	0.534523991
Standard Error	3465.335395
Observations	28

**ANOVA**

	df	SS	MS	F	Significance F
Regression	1	394458380	384458380	32.00513772	5.98698E-06
Residual	26	312330413	1201270813		
Total	27	696798753			

**Coefficients**

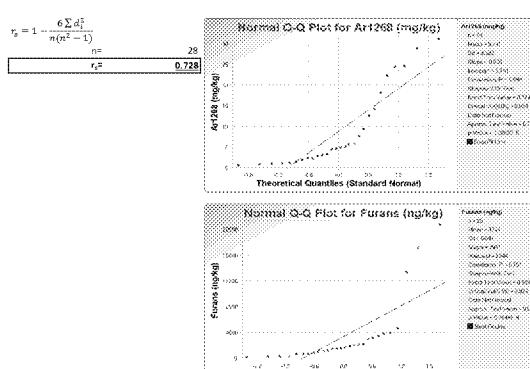
	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	-1712333681	902.8777988	0.189562873	0.851054	-2027.125263	-2027.125263	1684.658527
Arodror 1268 (mg/kg)	402.2073955	71.09518608	5.657098346	5.98608E-06	256.0691416	256.0691416	548.3456375

**Pearson Correlation Analysis**

Location	Log X	Log Y	(Log X)^2	(Log Y)^2	LOG X * LOG Y
D1-1A	0.4	3.1	1.129481574	9.94701231	1.10878905
D1-1B	0.7	3.2	0.503063878	10.33692319	2.280379938
D1-2A	0.1	2.8	0.016932513	7.571654743	0.376209095
D1-2B	0.4	2.8	0.129481574	7.197132632	0.997815144
D2-1A	0.5	3.6	0.231787005	12.840125998	1.725159221
D2-1B	0.5	3.5	0.257917586	12.249733056	1.774476184
EC-1A	0.7	3.0	0.425425289	8.997914673	1.956512319
EC-1B	0.7	3.0	0.436743138	9.004426587	1.983083937
EC-2A	1.1	3.3	1.210815337	10.595933004	3.639471218
EC-2B	0.8	2.4	0.567887427	5.767686313	1.779615762
EC-3A	1.4	3.6	1.926039303	12.06293368	4.56483988
EC-3B	1.3	4.3	1.307390595	19.63342564	5.806839994
EC-4A	1.5	4.3	2.125926433	17.519726267	5.176304131
EC-4B	0.9	3.5	0.781860617	12.512593834	3.17715932
LC-1A	0.1	2.0	0.020192389	8.132478024	0.046624984
LC-1B	0.0	2.5	0.020352541	13.04783823	0.055318886
MC-1A	1.0	3.3	0.942475184	11.02193125	3.222034785
MC-1B	0.5	3.1	0.209265956	9.915640443	1.437056019
MC-2A	0.7	3.2	0.486128756	10.11502452	2.21747701
MC-2B	1.2	3.3	1.327768429	11.02199125	3.825526368
MC-3A	0.8	3.1	0.569041412	9.81506969	2.352297727
MC-3B	1.3	3.3	1.575709065	10.70798554	4.107635555
PC-1A	1.5	4.1	2.228333579	17.00846463	6.156409639
PC-1B	1.4	3.7	1.92978241	13.4233947	5.089619924
PC-2A	0.1	2.8	0.008727611	7.509849144	0.262743389
PC-2B	0.0	2.3	0.000164794	5.360801523	0.029722546
PC-3A	0.3	2.5	0.076431129	6.249890939	0.631143968
PC-3B	-0.2	2.3	0.04744822	5.355932006	-0.5067473

**Spearman Correlation Analysis**

Location	Furan Rank	Arodror 1268 Rank	Rank Difference	Difference %
D1-1A	18	20.5	-2.5	12.5%
D1-1B	16	22	-1	5%
D1-2A	24	23	1	1%
D1-2B	23	20.5	2.5	12.5%
D2-1A	5	18	-13	169
D2-1B	8	17	-1	8%
EC-1A	20	16	4	26%
EC-1B	19	15	4	26%
EC-2A	12	8	4	36%
EC-2B	26	12	14	195%
EC-3A	6	4	2	4%
EC-3B	1	5	-4	16%
EC-4A	2	2	0	0%
EC-4B	7	10	-3	9%
LC-1A	21	27	-6	36%
LC-1B	9	26	-17	289%
MC-1A	10.5	9	1.5	22.5%
MC-1B	16	19	-3	9%
MC-2A	15	14	1	7%
MC-2B	10.5	7	3.5	12.5%
MC-3A	17	11	6	36%
MC-3B	13	6	7	49%
PC-1A	3	1	2	4%
PC-1B	4	3	1	1%
PC-2A	22	24	-2	4%
PC-2B	27	25	2	4%
PC-3A	25	22	3	9%
PC-3B	28	28	0	0%



Location	X: PCDD/F (ng/kg)	X: A1268 (ng/kg)
S5	27088	55
61	141965	5900
62	1442	590
1718	16468	55
BRO48	2861	1.4
C-15	10834	0.098
C-6	5048	756
C-8	1054	2.2
111	9396	6.1
EP4-E3	240288	3800
EP4-F2	5049	1188
EP4-H1	59263	4000
GRID MARS91	5900	5.2
117	2138	11
110	9048	0.25
109	855	1.1
101	2668	0.008
102	2678	0.13
D1-1A	8114	2.8
D1-1B	8044	5.12
D2-2A	885	3.97
D2-3A	5145	2.38
D2-3B	10471	5.03
D2-1B	8762	5.22
EC-1A	8527	4.49
EC-1B	7530	1.59
EC-2A	8868	12.5
EC-2B	5760	5.67
EC-3A	9544	24.4
EC-3B	5128	22.1
EC4-A	1217	2.68
EC-4B	9798	7.66
LC-1A	6889	0.721
LC-1B	15334	0.964
MC-1A	10588	3.35
MC-1B	10096	2.86
MC-2A	8594	4.98
MC-2B	8116	14.2
MC-3A	9010	5.68
MC-3B	5018	18
PC-1A	40766	51.1
PC-1B	18861	24.5
PC-2A	5534	1.24
PC-2B	5478	1.05
PC-3A	1801	1.89
PC-3B	1128	0.604

## Regression Analysis

## SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.91244098
R Square	0.83675730
Adjusted R Square	0.83652739
Standard Error	31970.40714
Observations	45

## ANOVA

	d.f.	SS	MS	F	Significance F
Regression	1	2.94894E+11	2.94894E+11	268.5162765	6.070356E-21
Residual	44	44972.05945	1021.06953		
Total	45	3.00877E+11			

## Coefficients

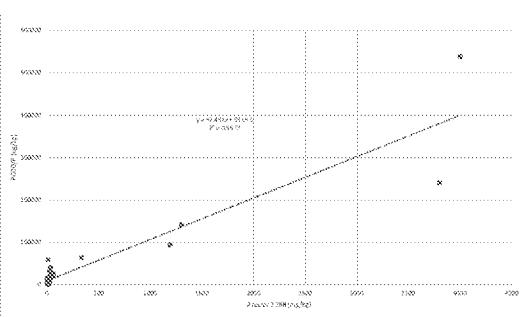
Intercept	Standard Error	t Stat	P-value	Lower 95%	Upper 95%
9512.33582	4909.87366	2.02032115	0.048457713	24.12979434	18614.54185
87.492222	5.739542072	16.98575688	6.07035621	85.92473368	109.0507107

## Pearson Correlation Analysis

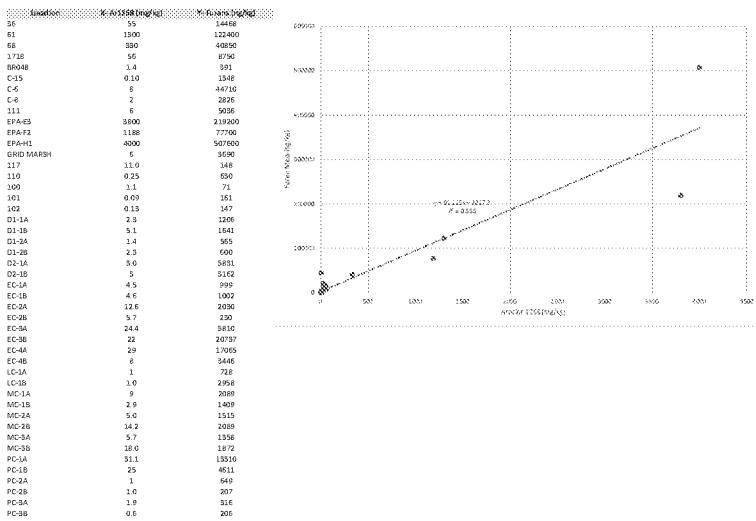
Location	X: PCDD/F (ng/kg)	X: A1268 (ng/kg)
S5	1.7	4.4
61	3.1	4.8
62	1.7	4.5
1718	0.1	3.5
BRO48	-0.1	4.0
C-15	-1.0	4.0
C-6	0.9	3.8
C-8	0.5	4.0
111	0.8	4.0
EP4-E3	3.5	5.4
EP4-F2	3.1	5.0
EP4-H1	3.6	5.7
GRID MARS91	0.6	1.8
117	1.0	3.3
110	-0.6	3.5
100	0.0	2.9
101	-1.1	3.3
102	-0.9	3.4
DC-25	-0.4	3.9
D1-1B	0.7	4.0
D1-2A	0.1	3.8
D2-1B	0.4	4.0
D2-2A	0.5	4.0
D2-3A	0.5	3.9
EC-1A	0.7	3.9
EC-1B	0.7	3.9
EC-2A	1.1	4.0
EC-2B	0.8	3.6
EC-3A	1.5	4.0
EC-3B	1.5	4.0
EC-4B	1.5	4.5
EC-5B	0.9	4.0
LC-1A	-0.1	3.8
LC-1B	0.0	4.2
MC-1A	1.0	4.0
MC-1B	0.5	4.0
MC-2A	0.7	3.9
MC-2B	1.2	4.0
MC-3A	0.8	3.7
MC-3B	1.5	3.8
PC-1A	1.5	4.5
PC-1B	1.4	4.3
PC-2A	0.1	3.5
PC-2B	0.0	3.5
PC-3A	0.5	3.2
PC-3B	-0.2	3.1

## Spearman Correlation Analysis

Location	PCDD/F Rank	A1268 Rank	Rank Difference	Significance
S5	9	2	1	
61	3	0	0	
62	5	0	0	
1718	11	6	5	
BRO48	40	35	5	
C-15	14	30	-16	
C-6	6	19	-13	
C-8	19	33	-14	
111	21	20.5	-0.5	
EP4-E3	2	2	0	
EP4-F2	4	4	0	
EP4-H1	1	1	0	
GRID MARS91	34	20.5	13.5	
117	42	15	26	
110	38	25	-3	
100	45	38	-3	
101	49	45	-4	
102	41	44	-3	
D1-1A	28	31.5	-3.5	
D1-1B	24	11	0	
D1-2A	30	55	-25	
D1-2B	32	51.5	-0.5	
D2-1A	16	29	-13	
D2-1B	25	28	-3	
EC-1A	27	27	0	
EC-1B	26	3	9	
EC-2A	19	15	4	
EC-2B	26	29	-3	
EC-3A	22	11	11	
EC-3B	8	12	-4	
EC-4A	20	9	1	
EC-4B	20	18	-2	
LC-1A	51	41	10	
LC-1B	33	40	-7	
MC-1A	17	17	0	
MC-1B	18	90	-72	
MC-2A	26	25	1	
MC-2B	23	11	9	
MC-3A	31	22	13	
MC-3B	33	15	20	
PC-1A	7	8	-1	
PC-1B	12	10	2	
PC-2A	57	57	0	
PC-2B	58	39	-1	
PC-3A	44	34	10	
PC-3B	45	42	3	



H<sub>0</sub> = PCDD/F not correlated to Aroclor 1268  
H<sub>a</sub> = PCDD/F correlated to Aroclor 1268  
p<0.05  
Status: PCDD/F correlated to Aroclor 1268



## Regression Analysis

## SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.951684686
R Square	0.86799068
Adjusted R Square	0.86499067
Standard Error	500.04 6145
Observations	46

## ANOVA

	d.f.	SS	F	Significance F
Regression	1	2,632,536.411	2,632,536.411	289,331,029.95
Residual	44	40057,4087	908903956.1	
Total	45	3,032,936.111		

## Coefficients

	Intercept	Standard Error	t Stat	P-value	Lower 95.0%	Upper 95.0%
Aroclor 1268 (mg/kg)	2817,328,495	4632,550728	60,6615,91232	0,544,20395,28	-5318,86405	11,155,61052

## Residuals

Intercept	Aroclor 1268 (mg/kg)
92,115,932,98	5,415,448,73

## Pearson Correlation Analysis

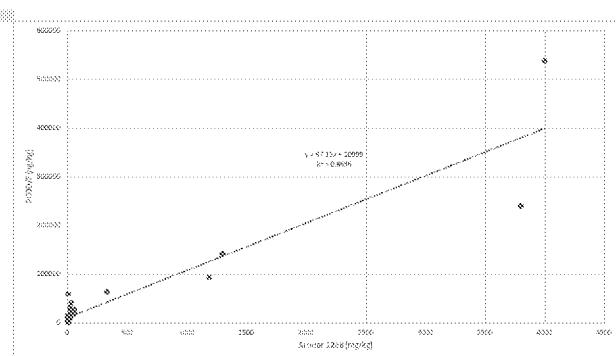
Location	Log(X)	Log(Y)	Log(X)*Log(Y)	Log(X)^2	Log(Y)^2
36	1.7	4.2	5.021862291	17,308,99887	7,14001,972
61	5.1	5.1	9,694,545402	25,889,51971	15,849,05113
65	2.5	4.6	5,843,912405	21,105,91113	11,135,145
1718	1.7	3.9	5,195,031379	15,559,42425	6,617,3294
BFO48	0.1	2.5	0,021350403	6,715,30305	0,376,9698
C-15	-1.0	3.1	1,008,744662	9,749,598924	1,181,75861
C-6	0.9	4.7	7,779,817911	31,905,65924	10,187,0855
C-8	0.3	5.5	0,117,932,02	31,905,65924	10,187,0855
111	0.9	5.7	12,974,981818	32,592,75635	10,187,0855
EPA-E3	3.6	5.5	12,614,5566	28,524,5778	10,187,0855
EPA-F2	3.1	4.9	9,454,481344	23,915,6174	10,187,0855
EPA-H1	3.6	5.7	12,974,981818	32,592,75635	10,187,0855
GRID MARSH	0.8	3.5	0,651,74295	12,735,7707	8,801,29221
117	1.0	2.2	1,008,744662	4,725,7707	4,725,7707
110	-0.6	1.8	0,583,476233	7,563,67512	4,685,57047
100	0.0	1.8	0,901,713054	9,419,03012	0,079,01511
101	-1.1	2.2	1,141,448387	4,712,59525	-3,362,71820
102	-0.9	2.2	0,785,695833	4,707,67934	-1,921,28079
114	-0.4	1.1	0,123,615134	3,117,95925	-1,777,95925
D1-1B	0.7	3.2	0,501,658568	10,330,62319	2,203,79988
D1-2A	0.1	3.8	0,015,982515	7,517,58475	0,375,020955
D1-2B	0.4	3.8	0,120,481574	7,517,58475	0,999,71544
D1-3B	0.0	3.5	0,923,600000	12,735,7707	4,725,7707
D3-1B	0.5	3.5	0,25,793,586	12,249,73506	1,777,47184
EC-1A	0.7	3.0	0,421,4243289	8,979,14675	1,955,61210
EC-1B	0.7	3.0	0,456,743138	9,044,04687	1,869,08397
EC-2A	1.1	3.5	1,216,013307	10,895,90005	1,634,71212
EC-2B	0.0	3.5	0,943,74437	5,530,69303	3,720,27925
EC-3A	1.4	3.5	1,349,759455	11,021,93125	5,625,93598
EC-3B	1.3	4.5	1,807,935986	12,825,93598	4,981,3869
EC-4A	1.5	4.2	1,216,924438	17,910,73767	6,175,90413
EC-4B	0.9	3.5	0,781,470107	11,512,90154	1,177,95925
LC-1A	-0.1	3.9	0,021,350399	8,110,73705	-0,302,65834
LC-1B	0.0	3.5	0,006,235541	12,047,92329	-0,052,63935
MC-1A	1.0	3.5	0,942,475184	11,021,93125	5,235,04745
MC-1B	0.5	3.1	0,206,629954	9,935,66045	1,457,05019
MC-2A	0.7	3.2	0,483,759479	10,402,91019	2,117,07070
MC-2B	1.2	5.3	1,321,759428	11,021,93125	5,625,93598
MC-3A	0.8	3.1	0,569,041412	9,915,60962	2,353,97727
MC-5B	1.3	3.3	1,579,041602	10,150,98554	4,107,93595
PC-1A	1.5	4.1	2,233,353379	17,000,63179	6,313,95925
PC-1B	1.4	3.7	1,837,93541	15,423,5447	5,089,1934
PC-2A	0.1	2.8	0,009,727,611	7,909,69144	0,252,7423869
PC-2B	0.6	2.5	0,006,150,784	5,540,61523	0,027,72545
PC-3A	0.3	2.5	0,076,451,129	6,249,09329	0,681,143898
PC-3B	-0.2	2.3	0,04,794,022	5,555,89206	-0,506,74575

## Spearman Correlation Analysis

Location	Aroclor 1268 (mg/kg)	Furan (mg/kg)	Rank Correlation	Correlation Coefficient
36	7	9	-2	4
61	5	5	0	0
65	5	6	-1	1
1718	6	11	-5	25
BFO48	55	38	-5	9
C-15	25	29	15	255
C-6	19	5	14	196
C-8	33	20	13	169
111	20.5	12	8.5	72.35
EPA-E3	2	2	0	0
EPA-F2	1	1	0	0
GRID MARSH	20.5	16	4.5	20.25
117	16	44	-28	784
110	45	55	8	64
100	38	48	-8	54
101	46	43	3	9
102	44	45	-1	1
D1-1A	31.5	30	1.5	2.25
D1-1B	24	25	-1	1
D1-3A	55	56	-4.5	20.35
D2-1A	29	14	15	225
D2-1B	28	18	10	100
D3-1B	27	32	-5	25
EC-1B	26	31	5	25
EC-2A	15	19	-6	64
EC-2B	23	40	-17	269
EC-3A	11	15	-4	16
EC-3B	12	7	5	25
EC-4A	18	17	1	1
LC-1A	41	35	8	64
LC-1B	40	21	-21	461
MC-1A	17	21.5	-4.5	20.35
MC-1B	30	27	0	9
MC-2A	25	26	-1	1
MC-2B	14	21.5	-7.5	56.25
MC-3A	22	18	-5	35
MC-3B	15	24	-11	121
PC-1A	8	10	-2	4
PC-1B	10	13	-3	9
PC-2A	97	94	8	9
PC-2B	20	21	4	4
PC-3A	34	39	-5	25
PC-3B	42	42	0	0

Case 3a: Co-location of PCDD/F Concentration and Aroclor 1268 (Original Distribution)

Location	Y-PCDD/F (ng/kg)	X-Ar1268 (ng/kg)
39	27038	55
61	141906	1300
68	64192	330
1718	18409	59
BR0446	2981	14
C-15	10524	0.099
C-6	58189	7.58
111	9296	6.1
EPA-E3	240328	3600
EPA-F2	94065	1188
EPA-H1	315204	4000
GRD MARSH	5980	0.1
117	2133	11
110	3049	0.25
100	856	1.1
101	2058	0.085
102	2678	0.13
D2-1A	10471	3.03
D2-1B	8762	3.22
EC-3A	9344	24.4
EC-3B	31225	22.3
EC-4A	18257	28.8
EC-4B	9796	7.66
LC-3A	6639	0.721
LC-1B	15394	0.964
PC-1A	40760	31.1
PC-1B	18361	24.5
PC-2A	3534	1.24
PC-2B	3477	1.03
PC-3A	1691	1.89
PC-3B	1120	0.604
D1-2A	6945	1.37
D1-2B	6285	2.29

Regression Analysis  
SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.929288027
R Square	0.863375236
Adjusted R Square	0.851654291
Standard Error	36015.98318
Observations	33

H<sub>0</sub> = PCDD/F not correlated to Aroclor 1268  
H<sub>a</sub> = PCDD/F correlated to Aroclor 1268  
p<0.05  
Status: PCDD/F correlated to Aroclor 1268

## ANOVA

	df	SS	MS	F	Significance F
Regression	1	2.03599E+11	2.03599E+11	196.2331389	5.93396E-15
Residual	31	44501654291	1455214597		
Total	32	3.28401E+11			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%
Intercept	10996.59331	7094.20235	1.570284916	0.124501041	-3268.571562	25263.75818
Ar1268 (ng/kg)	97.15010107	6.9305169523	14.00832391	5.93396E-15	83.00572956	111.2944726

## Pearson Correlation Analysis

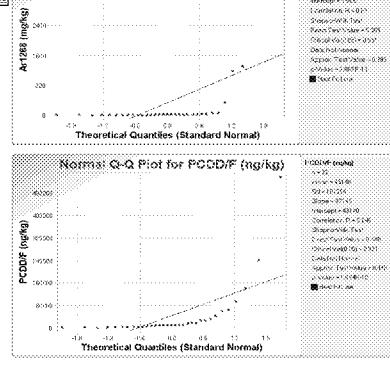
Location	PCDD/F	Ar1268	PCDD/F x Ar1268
36	1.7	4.4	3.012884251
61	3.1	5.2	9.659645201
68	2.5	4.8	6.342912465
1718	1.7	4.2	3.0516101378
BR0446	0.1	3.5	0.021353403
C-15	-1.0	4.0	1.006746682
C-6	0.9	4.8	0.770257509
111	0.6	4.0	0.616794295
EPA-E3	3.6	5.4	12.3146506
EPA-F2	3.1	5.0	9.45496144
EPA-H1	3.6	5.7	12.97403018
GRD MARSH	0.6	3.8	0.616794295
117	1.0	3.3	1.06496725
110	-0.6	3.5	0.624762323
100	0.0	2.9	0.001713354
114	-1.1	3.5	1.14070721
102	-0.5	3.4	0.755964363
D2-1A	0.5	4.0	0.211787605
D2-1B	0.5	3.9	0.25793756
EC-3A	1.4	4.0	1.92485053
EC-3B	1.3	4.5	1.807905056
EC-4A	1.5	4.4	2.12620643
EC-4B	0.9	4.0	0.781660517
C-1A	-0.1	3.2	0.00027721
C-1B	0.0	4.2	0.000235541
PC-1A	1.5	4.6	2.226332579
PC-1B	1.4	4.3	1.92797241
PC-2A	0.1	3.5	0.008727611
PC-2B	0.0	3.5	0.00164794
PC-3A	0.3	3.2	0.079431129
D1-2A	0.1	3.6	0.018692513
D1-2B	0.4	3.6	0.124981574

## Spearman Correlation Analysis

Location	PCDD/F Rank	Ar1268 Rank	Rank Difference	Significance
36	9	7	2	4
61	3	3	0	0
68	5	5	0	0
1718	11	6	5	25
BR0446	27	22	5	25
C-15	14	32	-16	324
C-6	6	15	-9	31
111	17	10.5	0.5	0.25
EPA-E3	2	2	0	0
EPA-F2	4	4	0	0
EPA-H1	1	1	0	0
GRD MARSH	23	16.5	6.5	42.25
117	29	13	16	256
110	26	30	4	16
100	33	25	8	64
101	30	33	-3	9
102	28	31	-2	9
D2-1A	15	19	-4	16
D2-1B	19	10	1	1
EC-3A	16	11	7	49
EC-3B	8	12	-4	16
EC-4A	10	9	1	1
EC-4B	16	14	2	4
LC-3A	21	28	-7	49
PC-1A	7	8	-1	1
PC-1B	12	10	2	4
PC-2A	24	24	0	0
PC-2B	25	16	4	1
PC-3A	31	21	10	100
PC-3B	32	29	3	9
D1-2A	20	23	-3	9
D1-2B	22	20	2	4

$$t_p = 1 - \frac{6 \sum d_i^2}{n(n^2 - 1)}$$

n= 32  
t\_p = 0.780



$$\text{PCCDF}(\text{mg/kg})$$

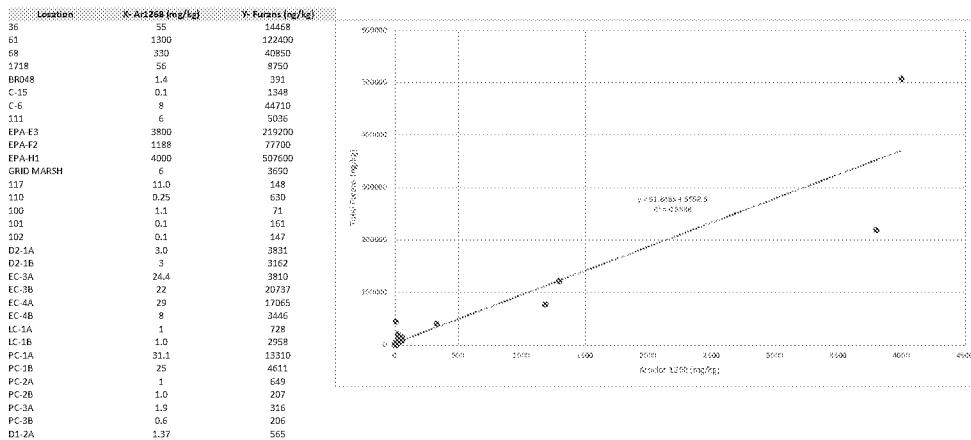
n=32  
Mean=2000  
SD=1000  
Skewness=-0.08  
Kurtosis=3.03  
PValue>0.05  
D>0.05  
PValue>0.05  
Shapiro-Wilk Test  
Z>1.96  
PValue<0.05  
D>0.05  
PValue>0.05  
Anderson-Darling Test  
A>0.72  
PValue<0.05  
D>0.05  
PValue>0.05

Normal Q-Q Plot for PCDD/F (mg/kg)

$$\text{PCCDF}(\text{mg/kg})$$

n=32  
Mean=2000  
SD=1000  
Skewness=-0.08  
Kurtosis=3.03  
PValue>0.05  
D>0.05  
PValue>0.05  
Shapiro-Wilk Test  
Z>1.96  
PValue<0.05  
D>0.05  
PValue>0.05  
Anderson-Darling Test  
A>0.72  
PValue<0.05  
D>0.05  
PValue>0.05

**Case 3b: Co-location of Furan Mass and Aroclor 1268 (Original Distribution)**



**Regression Analysis**  
**SUMMARY OUTPUT**

Regression Statistics	
Multiple R	0.929419365
R Square	0.863820356
Adjusted R Square	0.859427465
Standard Error	35994.05431
Observations	33

**ANOVA**

	df	SS	MS	F	Significance F
Regression	1	2.53489E+11	2.53489E+11	196.6404842	5.77075E-15
Residual	31	3996213496	1289101116		
Total	32	2.93452E+11			

**Coefficients**

	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	6658.259321	60.01509293	0.553023119	0.58421401	-983.27166	17148.8703	17148.8703
Aroclor 1268 (mg/kg)	91.84823482	6.545985133	14.03285975	5.77075E-15	78.48963563	105.206834	105.206834

**Significance**

Location	Log X	Log Y	Log X^2	Log Y^2	LOG X * LOG Y
36	1.7	4.2	3.02882291	17.30898987	7.240613722
61	3.1	5.1	9.656643201	25.8851971	15.84306311
68	2.5	4.6	6.342912465	21.26302913	11.65335146
1718	1.7	3.9	3.056161378	15.5394275	6.891371284
BR048	0.1	2.6	0.021353403	6.71938035	0.37878968
C-15	-1.0	3.1	1.00874862	9.794958832	3.143350381
C-6	0.9	4.7	0.773817911	21.62626395	4.09981778
111	0.8	3.7	0.61674295	13.70540941	2.907363855
EPA-E3	3.6	5.3	12.8148506	28.52457778	19.11905339
EPA-F2	3.1	4.9	9.454459514	23.91621774	15.03714695
EPA-H1	3.6	5.7	12.57483618	32.55297688	20.55161313
GRID MARSH	0.8	3.6	0.61674295	12.72367703	2.802592221
117	1.0	2.2	1.084498725	4.70503774	2.585895179
110	-0.6	2.8	0.362476233	7.836307512	-1.685370947
100	0.0	1.8	0.000713354	3.415803012	0.07650151
101	-1.1	2.2	1.146543837	4.871258895	-2.362871829
102	-0.9	2.2	0.765093683	4.705767893	-1.921286279
D2-1A	0.5	3.6	0.231707008	17.30898987	1.72217221
D2-1B	0.05	3.5	0.237091285	12.24913306	1.774731614
EC-3A	1.4	3.6	1.92465053	12.823023268	4.50813988
EC-3B	1.3	4.3	1.807329586	18.6342954	5.302392913
EC-4A	1.5	4.2	2.129826433	17.01072367	6.176304131
EC-4B	0.9	3.5	0.781860517	12.512593934	3.127795932
LC-1A	-0.1	2.9	0.020182389	8.192478924	-0.406624884
LC-1B	0.0	3.5	0.009253541	12.04782929	-0.052689596
PC-3A	1.5	4.1	2.28333579	17.00884463	6.156409639
PC-3B	1.4	3.7	1.92978241	13.4233947	0.985613924
PC-2A	0.1	2.8	0.008727611	7.909840144	0.26743389
PC-2B	0.0	2.3	0.000164754	5.360801523	0.029722545
PC-3A	0.3	2.5	0.076431129	6.249809329	0.69143956
PC-3B	-0.2	2.3	0.04794482	5.355932006	-0.50674373
D1-2A	0.1	2.8	0.018692513	7.571654473	0.376209055
D1-2B	0.4	2.8	0.129481574	7.719732632	0.999781544

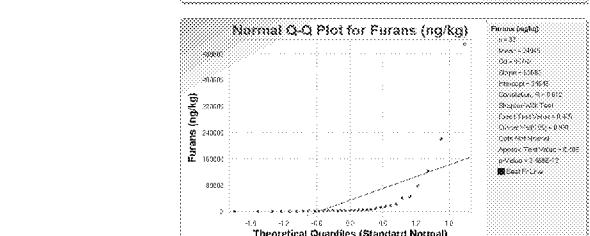
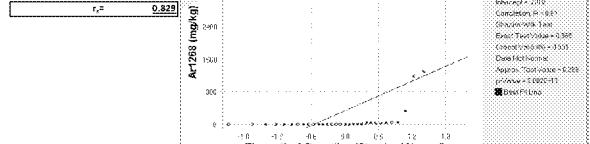
**Spearman Correlation Analysis**

Location	Aroclor 1268 Rank	Furans Rank	Rank Difference	Difference^2
36	7	9	-2	4
61	3	3	0	0
68	5	8	-1	1
1718	6	11	-5	25
BR048	22	26	-4	16
C-15	32	20	12	144
C-6	15	5	10	100
111	16.5	12	4.5	20.25
EPA-E3	2	2	0	0
EPA-F2	4	4	0	0
EPA-H1	1	1	0	0
GRID MARSH	16.5	16	0.5	0.25
117	13	31	-18	324
110	30	23	7	49
100	25	33	-8	64
101	33	35	3	9
102	31	32	-1	1
D2-1A	19	14	5	25
D2-1B	18	18	0	0
EC-2A	11	15	-4	16
EC-3B	12	7	5	25
EC-4A	9	8	1	1
EC-4B	14	17	-3	9
LC-1A	28	21	7	49
LC-1B	27	19	8	64
PC-3A	8	10	-2	4
PC-3B	10	13	-3	9
PC-2A	24	22	2	4
PC-2B	26	28	-2	4
PC-3A	21	27	-6	36
PC-3B	29	29	0	0
D1-2A	23	25	-2	4
D1-2B	20	24	4	16

$$r_s = 1 - \frac{6 \sum d_i^2}{n(n^2 - 1)}$$

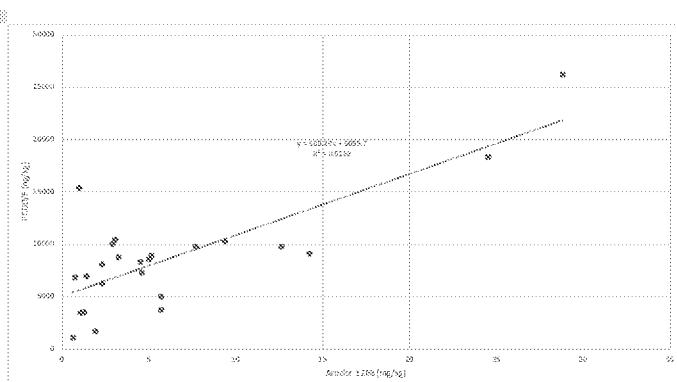
n= 33

$r_s^2 = 0.829$



Case 1a: Co-location of PCDD/F Concentration and Aroclor 1268, Excluding Outliers (Co-location Study Data)

Location	Y-PCDD/F (ng/kg)	X-Ar1268 (mg/kg)
D1-1A	8114.0	2.29
D1-1B	8943.5	5.12
D1-2A	6944.9	1.37
D1-2B	6285.4	2.29
D2-1A	10470.6	3.03
D2-1B	8762.1	3.22
EC-1A	8337.3	4.49
EC-1B	7319.9	4.58
EC-2A	9893.0	1.24
EC-2B	3700.8	5.67
EC-4A	2657.2	28.6
EC-4B	5798.3	7.68
LC-1A	6288.7	0.721
LC-1B	15333.8	0.964
MC-1A	10308.4	9.39
MC-1B	10040.3	2.88
MC-2A	8594.3	4.98
MC-2B	9115.8	14.2
MC-3A	5032.9	5.68
PC-1B	18360.8	24.5
PC-2A	3534.4	1.24
PC-2B	3473.3	1.03
PC-3A	1691.0	1.89
PC-3B	11276.6	0.604



#### Regression Analysis SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.285279379
R Square	0.016920769
Adjusted R Square	0.0598402531
Standard Error	3415.177045
Observations	24

H<sub>0</sub> = PCDD/F not correlated to Aroclor 1268  
H<sub>1</sub> = PCDD/F correlated to Aroclor 1268  
p<0.05  
Status: PCDD/F correlated to Aroclor 1268

#### ANOVA

	df	SS	MS	F	Significance F
Regression	1	413053353.4	413053353.4	3541438523	5.66379E-06
Residual	22	265659553.5	11653434.25		
Total	23	669648906.9			

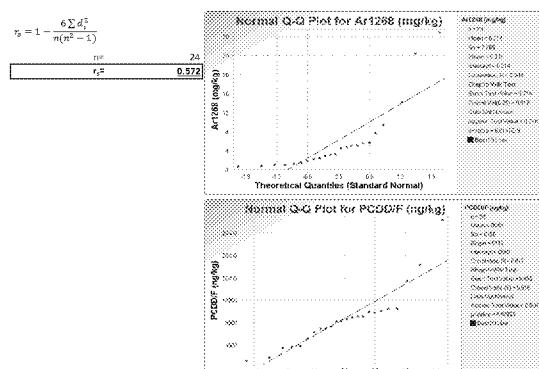
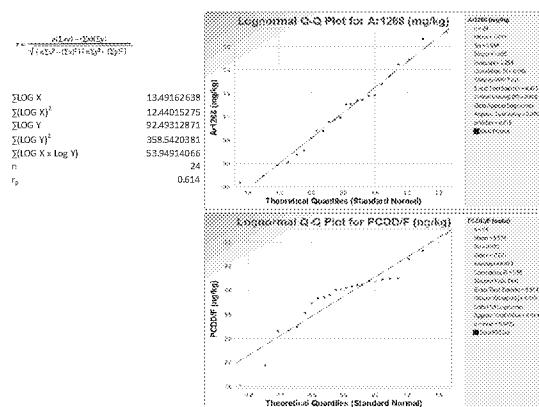
#### Pearson Correlation Analysis

Location	Log X	Log Y	(Log X) <sup>2</sup>	(Log Y) <sup>2</sup>	LOG X * LOG Y
D1-1A	0.4	3.9	0.129481574	15.28211831	1.406681463
D1-1B	0.7	4.0	0.503063878	15.61441161	2.820285578
D1-2A	0.1	3.8	0.025200000	14.4277638	0.252520000
D1-2B	0.4	3.8	0.129481574	14.4277638	1.365744859
D2-1A	0.5	4.0	0.231797055	16.160377141	1.935385679
D2-1B	0.5	3.9	0.257917586	15.55196817	2.020779892
EC-1A	0.7	3.9	0.402542528	15.37444041	2.557474489
EC-1B	0.7	3.9	0.43674319	14.394400094	2.5152318042
EC-2A	1.1	4.0	1.210815337	15.33904669	4.391973983
EC-2B	0.8	3.6	0.567887427	12.7212332	2.6942184
EC-4A	1.5	4.4	2.129826433	19.52075653	5.49421934
EC-4B	0.9	4.0	0.781860517	15.32928417	3.529093031
LC-1A	-0.1	3.8	0.020192398	14.70702215	-0.5448154503
LC-1B	0.0	4.2	0.000253541	17.53386518	-0.066674965
MC-1A	1.0	4.0	0.942475184	16.10570411	3.896526574
MC-1B	0.5	4.0	0.208269596	16.01397657	1.826216262
MC-2A	0.7	3.9	0.486528756	15.47801233	2.743047008
MC-2B	1.2	4.0	1.327788429	15.57997476	4.552825381
MC-3A	0.8	3.7	0.569041412	13.70245874	2.792460475
PC-1B	1.4	4.3	1.92578241	18.18077158	5.923273598
PC-2A	0.1	3.5	0.008727611	12.5905443	0.314689632
PC-2B	0.0	3.5	0.000164794	12.53685601	0.045453304
PC-3A	0.3	3.2	0.076431125	10.42091115	0.892458406
PC-3B	-0.2	3.1	0.047944822	9.31580021	-0.668306687

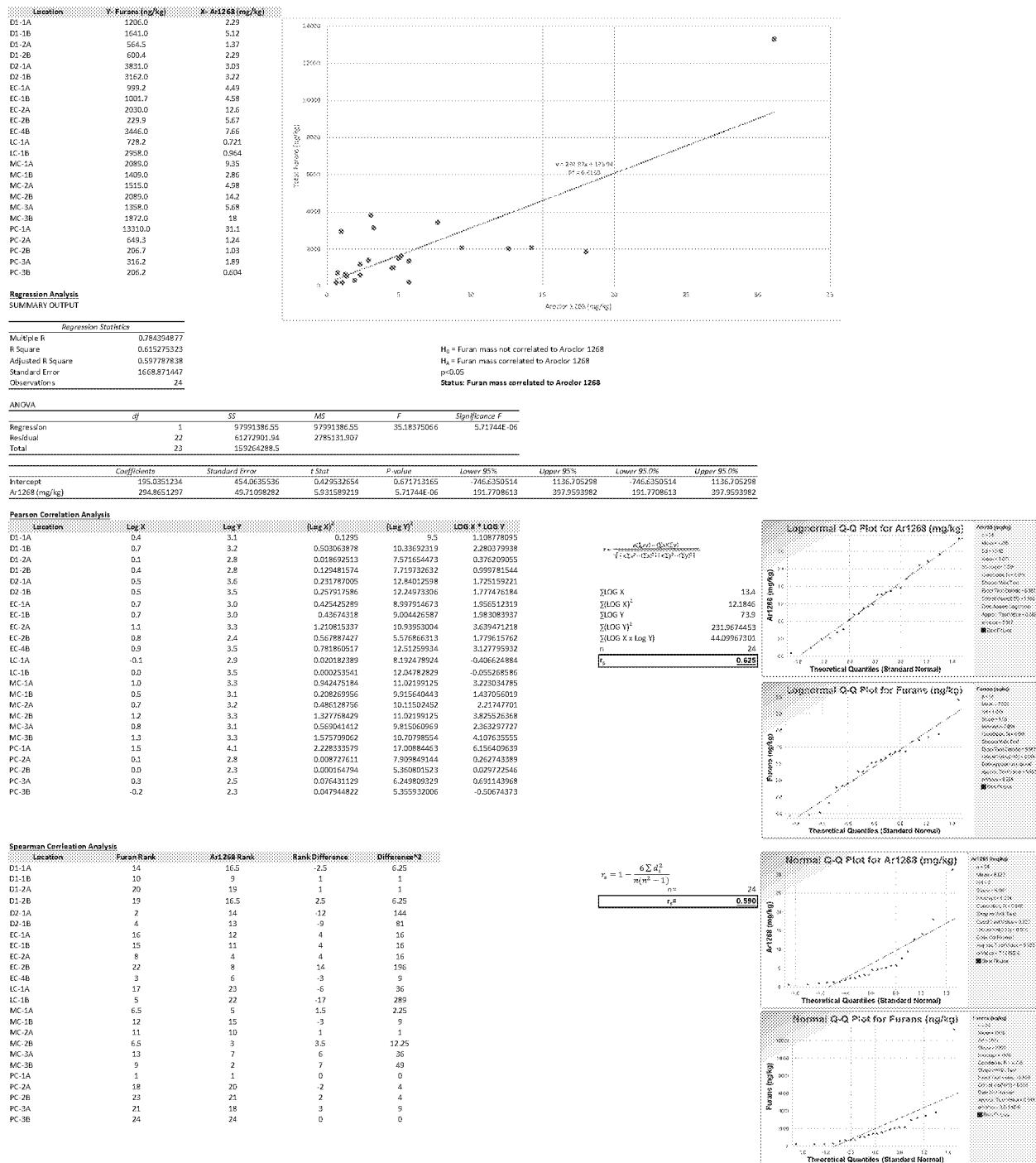
Pearson Correlation not applicable- variables not normally/ lognormally distributed

#### Spearman Correlation Analysis

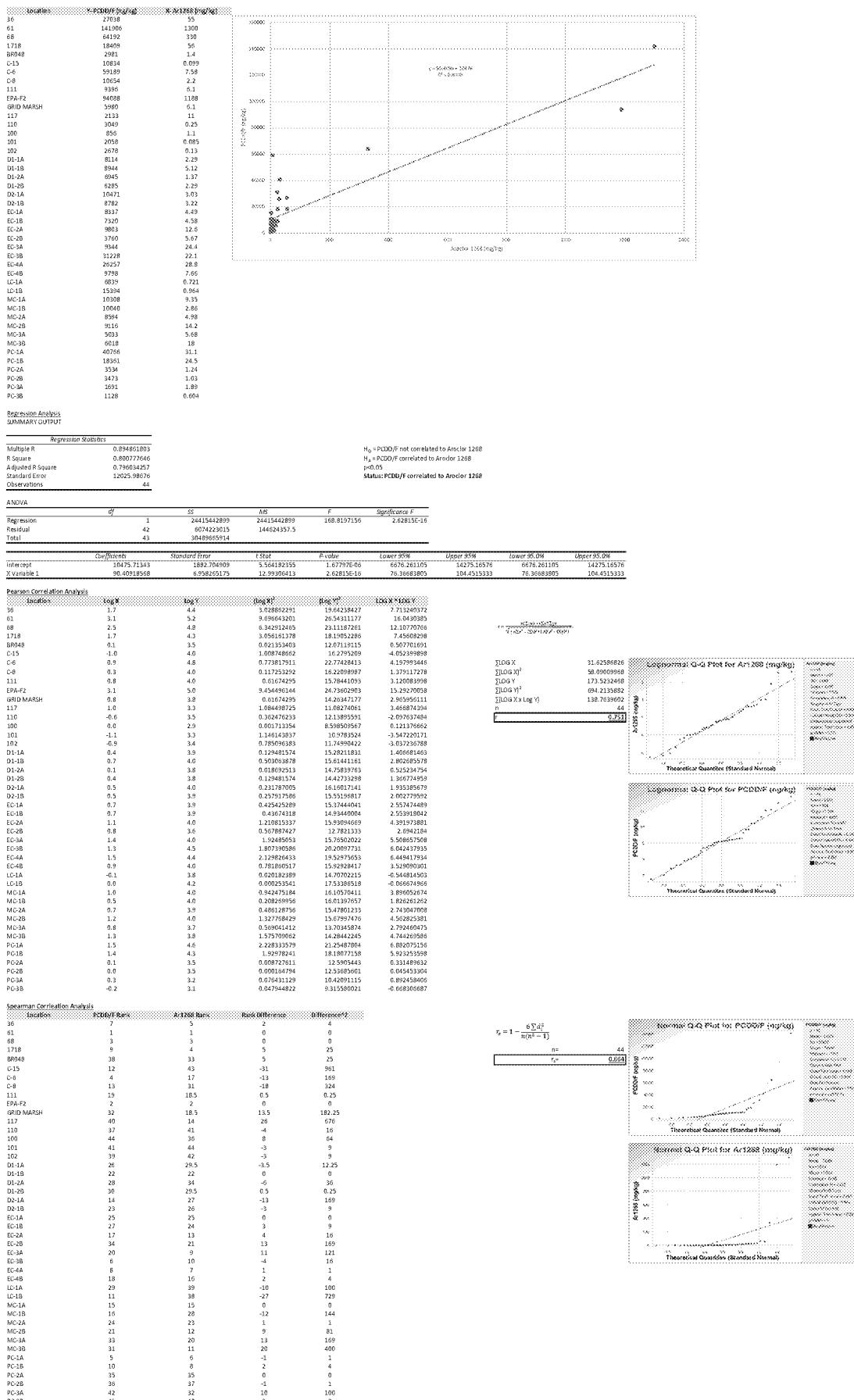
Location	FisherRank	Ar1268 Rank	Rank Difference	Difference <sup>2</sup>
D1-1A	14	16.5	-2.5	6.25
D1-1B	10	9	1	1
D1-2A	16	19	-3	9
D1-2B	18	16.5	1.5	2.25
D2-1A	4	14	-10	100
D2-1B	11	13	-2	4
EC-1A	13	12	1	1
EC-1B	15	11	4	16
EC-2A	7	4	3	9
EC-2B	20	8	12	144
EC-4A	1	1	0	0
LC-1A	6	5	2	4
LC-1B	17	23	-6	36
MC-1A	3	22	-19	361
MC-1B	5	5	0	0
MC-1B	6	15	-9	81
MC-2A	12	10	2	4
MC-2B	9	3	6	36
MC-3A	19	7	12	144
PC-1B	2	2	0	0
PC-2A	21	20	1	1
PC-2B	22	21	1	1
PC-3A	23	18	5	25
PC-3B	24	24	0	0



**Case 1b: Co-location of Furan Congener Concentration and Aroclor 1268, Excluding Outliers (Co-location Study Data)**

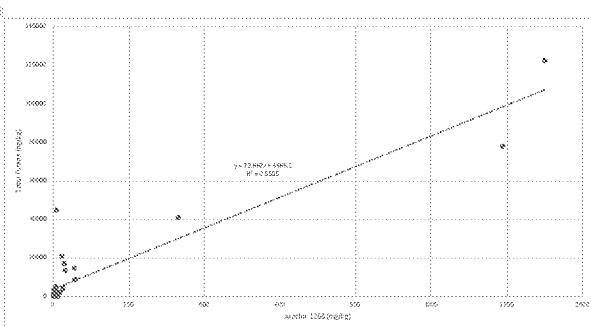


**Case 2a: Co-location of PCDD/F Concentration and Aroclor 1268, Excluding Outliers (Cumulative Data Set)**



**Case 2b: Co-location of Furan Congener Concentration and Aroclor 1268, Excluding Outliers (Cumulative Data Set)**

Location	X (log X)	X (X1268 mg/kg)	X (X1268 mg/kg) (%)
36	14408	55	
61	122400	1300	
68	4050	330	
1718	8750	56	
BR948	391	1.4	
C-15	1348	0.1	
C-6	44710	8	
C-8	2846	2	
111	5636	6	
EPA-F2	77200	1188	
GRID MARSII	3690	6	
117	148	11.0	
119	630	0.25	
100	71	1.1	
101	161	0.1	
102	147	0.1	
D1-1A	1205	2.3	
D1-1B	1641	5.1	
D1-2A	565	1.4	
D1-2B	609	2.3	
D2-1A	3152	3.0	
D2-1B	1099	4.5	
EC-1A	1002	4.6	
EC-2A	2030	12.6	
EC-2B	230	5.7	
EC-3A	3810	24.4	
EC-3B	2012	22	
EC-4A	17655	39	
EC-4B	3446	8	
LC-1A	728	1	
LC-1B	2958	1.0	
MC-1A	288	9	
MC-1B	1409	2.8	
MC-2A	3515	5.0	
MC-2B	2089	14.2	
MC-3A	1358	5.7	
MC-3B	3872	18.0	
PC-1A	15340	31.1	
PC-1B	4611	29	
PC-2A	649	1	
PC-2B	267	1.0	
PC-3A	318	1.9	
PC-3B	205	0.6	



**Regression Analysis  
SUMMARY OUTPUT**

Regression Statistics	
Multiple R	0.926537987
R Square	0.858472587
Adjusted R Square	0.855102866
Standard Error	8625.837656
Observations	44

**ANOVA**

	df	SS	MS	F	Significance F
Regression	1	18955604694	18955604694	254.7622541	1.938012E-15
Residual	42	3129013162	74405075.27		
Total	43	22080617955			

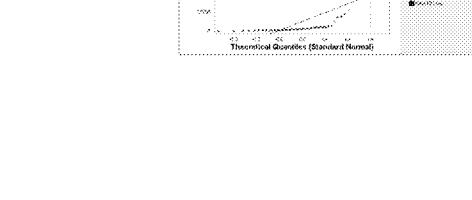
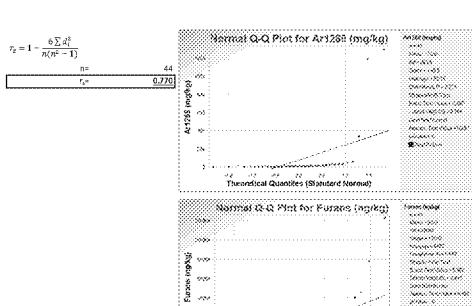
	Coefficients	Standard Error	tStat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	3665.237682	1350.401196	2.714194268	0.009598386	940.173737	6390.457627	940.173737	6390.457627
X Variable 1	79.66108032	4.99030039	15.96127357	1.936011619	69.58990351	89.73371512	69.58990351	89.73371512

**Pearson Correlation Analysis**

Location	log X	log Y	log X Y	log X X	log Y Y
36	1.7	4.2	7.240501722	17.38958887	17.240501722
61	3.1	5.1	9.096423201	25.89591971	15.84305311
68	2.5	4.6	8.342912485	21.626230921	11.01332015
1718	1.7	3.9	6.703520343	15.703520343	8.280520343
BR948	0.1	2.6	0.021353403	6.71593055	0.316780698
C-15	-1.0	3.1	1.008748662	9.794598983	-0.143595081
C-6	0.9	4.7	0.773817913	21.6262356	4.096817778
C-8	0.3	3.5	0.117253292	11.910580294	1.18759821
111	0.8	3.7	0.018692153	12.931621274	2.000725099
EPA-F2	5.1	4.9	9.8460944	23.91621409	13.07214609
GRID MARSII	0.8	3.6	0.01674295	12.232872753	2.001252223
117	1.0	2.2	0.004498725	4.705037734	2.258895347
119	-0.6	2.8	0.362476233	7.828307512	-1.085379947
100	0.0	1.8	0.00171354	3.415803012	0.076951051
101	-1.1	2.2	-0.00171354	4.397170247	-2.920520247
102	6.9	2.2	0.785650383	4.763761784	1.511285279
D1-1A	0.4	3.1	0.12481574	9.494701213	1.109770895
D1-1B	0.7	3.2	0.503053872	10.33692319	2.289379938
D1-2A	0.1	2.8	0.018692153	7.571054475	0.376295055
D1-2B	0.4	2.8	0.12481574	7.707325293	1.993146079
D2-1A	0.5	3.6	0.232179705	12.83695588	1.722152221
D2-1B	0.5	3.5	0.237917586	12.24973306	1.774741864
EC-1A	0.7	3.0	0.425425289	8.987914673	1.955123193
EC-1B	0.7	3.0	0.436743118	9.004425087	1.983053932
EC-2A	1.1	2.4	1.008748662	10.915644443	3.000071077
EC-2B	0.8	2.4	0.503053872	5.536805313	1.776117672
EC-3A	1.4	3.6	1.924895053	12.82302388	4.968110898
EC-3B	1.3	4.3	1.80739058	18.8342954	5.80339973
EC-4A	1.5	4.2	2.12882433	17.91072367	6.176304131
EC-4B	0.9	3.5	0.781809512	12.51259944	3.11779592
LC-1A	-0.1	2.3	0.002513541	1.04792829	-0.002513541
LC-1B	0.0	3.5	0.002513541	12.04792829	-0.053265858
MC-1A	1.0	3.3	0.942475184	11.012519235	3.220347895
MC-1B	0.5	3.1	0.202899556	9.915640444	1.437050619
MC-2A	0.7	3.2	0.488179756	10.11504525	2.127472701
MC-2B	1.2	3.3	0.503053872	10.33692319	3.022825078
MC-3A	0.8	3.3	0.569641412	9.815695985	2.363257227
MC-3B	1.3	3.3	1.575709062	10.7079854	4.107633555
PC-1A	1.5	4.1	2.288333579	17.00884465	6.156406035
PC-1B	1.4	3.7	1.92978247	13.4233947	5.088413924
PC-2A	0.1	2.3	0.002513541	2.94002442	-0.002513541
PC-2B	0.0	2.3	0.000154794	5.339801523	0.028725454
PC-3A	0.3	2.5	0.070431129	6.249890329	0.691143968
PC-3B	-0.2	2.3	0.04794482	5.355932006	-0.50674373

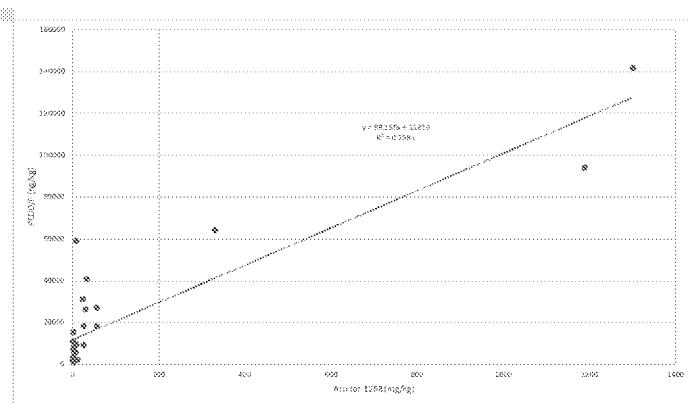
**Spearman Correlation Analysis**

Location	Aroclor 1268	Burden	Burden Rank	Burden Rank	Burden Rank
36	5	7	-2	4	
61	1	1	0	0	
68	3	4	-1	3	
1718	4	9	-5	25	
BR948	23	26	-3	9	
C-15	43	27	16	256	
C-6	17	3	14	196	
C-8	21	18	13	189	
111	18.5	10	8.5	72.25	
EPA-F2	2	2	0	0	
GRID MARSII	18.5	14	4.5	20.25	
117	14	42	-28	784	
119	41	33	8	64	
100	39	44	-8	64	
101	44	45	-3	9	
102	42	43	-1	1	
D1-1A	29.5	28	1.5	2.25	
D1-1B	22	23	-1	1	
D1-2A	34	35	-1	1	
D1-2B	25.5	34	-4.5	20.25	
D2-1A	27	12	15	225	
D2-1B	29	16	10	100	
EC-1A	25	30	-5	25	
EC-1B	24	29	-5	25	
EC-2A	13	21	-8	64	
EC-2B	21	38	-17	289	
EC-3A	9	13	-4	16	
EC-3B	10	5	5	25	
EC-4A	7	6	1	1	
EC-4B	10	15	1	1	
LC-1A	39	31	8	64	
LC-1B	38	17	21	441	
MC-1A	15	19.5	-4.5	20.25	
MC-1B	29	25	3	1	
MC-2A	23	32	-1	1	
MC-2B	12	19.5	-7.5	50.25	
MC-3A	20	28	-6	36	
MC-3B	11	22	-11	121	
PC-1A	6	8	-2	4	
PC-1B	8	11	-3	9	
PC-2A	33	30	3	9	
PC-2B	37	39	-2	4	
PC-3A	32	37	-5	25	
PC-3B	40	40	0	0	



**Case 3a: Co-location of PCDD/F Concentration and Aroclor 1268, Excluding Outliers (Original Distribution)**

Location	Y-PCDD/F (ng/kg)	X-Ar1268 (mg/kg)
36	27038	55
61	141906	1300
68	64192	330
1718	18409	56
BR048	2981	1.4
C-15	10834	0.099
C-6	59189	7.58
11	9395	5.1
EPA-F2	848898	1198
GRID MARSH	5889	5.1
117	2133	11
110	3049	0.25
100	856	1.1
101	2058	0.085
102	2679	0.13
D2-1A	10471	3.03
D2-1B	8782	3.22
EC-3A	9344	24.4
EC-3B	31228	22.1
EC-4A	26257	28.8
EC-4B	9798	7.68
LC-1A	6839	0.721
LC-1B	15394	0.964
PC-1A	40766	31.5
PC-1B	18361	24.5
PC-2A	3049	1.2
PC-2B	3472	1.03
PC-3A	1601	1.89
PC-3B	1128	0.604
D1-2A	6945	1.37
D1-2B	6295	2.29



**Regression Analysis SUMMARY OUTPUT**

Regression Statistics	
Multiple R	0.893339485
R Square	0.798055435
Adjusted R Square	0.79109183
Standard Error	1420343732
Observations	35

$H_0$  = PCDD/F not correlated to Aroclor 1268  
 $H_a$  = PCDD/F correlated to Aroclor 1268  
 $p < 0.05$

Status: PCDD/F correlated to Aroclor 1268

**ANOVA**

	df	SS	MS	F	Significance F
Regression	1	23119892311	23119892311	114.6037659	1.37521E-11
Residual	29	5850351320	201737631.7		
Total	30	28570283631			

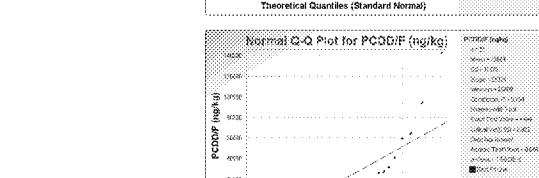
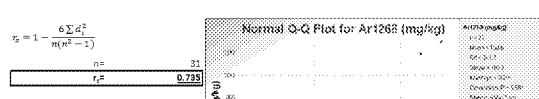
	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	11839.46177	2685.087013	4.402340205	0.002130408	6347.842219	17331.09132	6347.842219	17331.09132
Ar1268 (ng/kg)	89.155x2951	8.330967078	10.72531484	1.37921E-15	72.1468847	106.2243663	72.1468847	106.2243663

**Spearman Correlation Analysis**

Location	Log X	Log Y	(Log X)^2	(Log Y)^2	LOG X * LOG Y
36	1.7	4.4	3.028622931	19.54238427	7.713240372
61	3.1	5.2	9.696463201	26.5431157	16.0430385
68	2.5	4.8	6.342912465	23.1187261	12.10770765
1718	1.7	4.3	3.056161379	18.19052286	7.45608299
BR048	0.1	3.5	0.021354043	12.07119115	0.05701691
C-15	-1.0	4.0	1.009748662	16.2795209	-0.052399898
C-6	0.9	4.8	0.773817911	22.77428413	4.179593446
EPA-F2	3.1	5.0	9.454496144	24.7302903	15.29270058
GRID MARSH	0.8	3.8	0.651574295	14.2634717	3.965956111
117	1.0	3.3	1.084498725	11.08274063	3.46874394
110	-0.6	3.5	0.362476233	12.13895592	-2.076737484
100	0.0	2.9	0.001713594	8.8598509567	0.212378652
101	-1.1	3.3	1.146143837	10.9783524	-3.547230171
102	-0.9	3.4	0.785096383	11.749590422	-3.037236788
D2-1A	0.5	4.0	0.231707005	16.16917141	1.93558679
D2-1B	0.5	3.9	0.257917585	15.76301817	2.009745832
EC-3A	1.4	4.0	1.39205653	15.76301817	5.01065759
EC-3B	1.3	4.5	1.83039696	20.20997731	6.012413795
EC-4A	1.5	4.4	2.129326433	19.52975653	6.419417934
EC-4B	0.9	4.0	0.781860513	15.82284817	3.520949301
LC-1A	0.1	3.8	0.020392389	14.70702715	-0.544814503
LC-1B	0.0	4.2	0.002055841	17.53385518	-0.066674966
PC-1A	1.5	4.6	2.228333579	21.25487804	6.892075156
PC-1B	1.4	4.3	1.92798241	18.18077158	5.523275599
PC-2A	0.1	3.5	0.008727611	12.5905443	0.313486632
PC-2B	0.0	3.5	0.000164794	12.53685601	0.045453304
PC-3A	0.3	2.2	0.076431129	10.42091115	0.892458406
PC-3B	-0.2	3.1	0.04794482	9.315580021	-0.668306687
D1-2A	0.1	3.8	0.018692513	14.75839763	0.525234754
D1-2B	0.4	3.8	0.129481574	14.42733298	1.36674959

**Pearson Correlation Analysis**

Location	PCDD/F Rank	Ar1268 Rank	Rank Difference	Difference %
36	5	2	4	
61	1	0	0	
68	3	0	3	
1718	8	4	5	
BR048	25	20	5	
C-15	12	30	-18	324
C-6	4	13	.9	81
EPA-F2	2	2	0	0
GRID MARSH	21	14.5	6.5	42.25
117	27	11	16	256
110	24	28	-4	16
100	31	23	8	64
101	28	31	-.3	9
102	26	29	-.3	9
D2-1A	13	17	-.4	16
D2-1B	17	16	1	1
EC-3A	16	9	7	49
EC-3B	6	10	-.4	16
EC-4A	8	7	1	1
EC-4B	14	12	2	14
LC-1A	19	26	-.7	49
LC-1B	11	25	-.14	105
PC-1A	5	6	-.1	1
PC-1B	10	8	2	4
PC-2A	22	22	0	0
PC-2B	23	24	-.1	1
PC-3A	29	19	10	100
PC-3B	30	27	3	9
D1-2A	18	21	-.3	9
D1-2B	20	18	2	4



**Case 3b: Co-location of Furan Mass and Aroclor 1268, Excluding Outliers (Original Distribution)**

Location	Y-Furan (mg/kg)	X-Ar1268 (mg/kg)
36	1448	55
61	122400	1300
68	40859	330
1718	8750	56
BR048	391	1.4
C-15	1348	0.1
C-6	44710	8
11	5836	8
EPA-F2	177700	1188
GRID MARSH	3699	6
117	148	11.0
110	630	0.25
100	71	1.1
101	161	0.1
102	147	0.1
D2-1A	3831	30
D2-1B	3162	3
EC-3A	3810	24.4
EC-3B	20737	22
EC-4A	17065	29
EC-4B	3446	8
LC-1A	728	1
LC-1B	2958	1.0
PC-1A	13310	31.5
PC-1B	4611	25
PC-2A	649	1
PC-2B	207	1.0
PC-3A	316	1.9
PC-3B	206	0.6
D1-2A	565	1.37
D1-2B	600	2.29

Regression Analysis  
SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.92501242
R Square	0.85731381
Adjusted R Square	0.852393597
Standard Error	10145.2033
Observations	35

H<sub>0</sub> = Furan mass not correlated to Aroclor 1268  
H<sub>a</sub> = Furan mass correlated to Aroclor 1268  
p<0.05  
Status: Furan mass correlated to Aroclor 1268

ANOVA					
	df	SS	MS	F	Significance F
Regression	1	17934009093	17934009093	174,2432156	8.64297E-14
Residual	29	2984829349	102925150		
Total	30	20518838442			

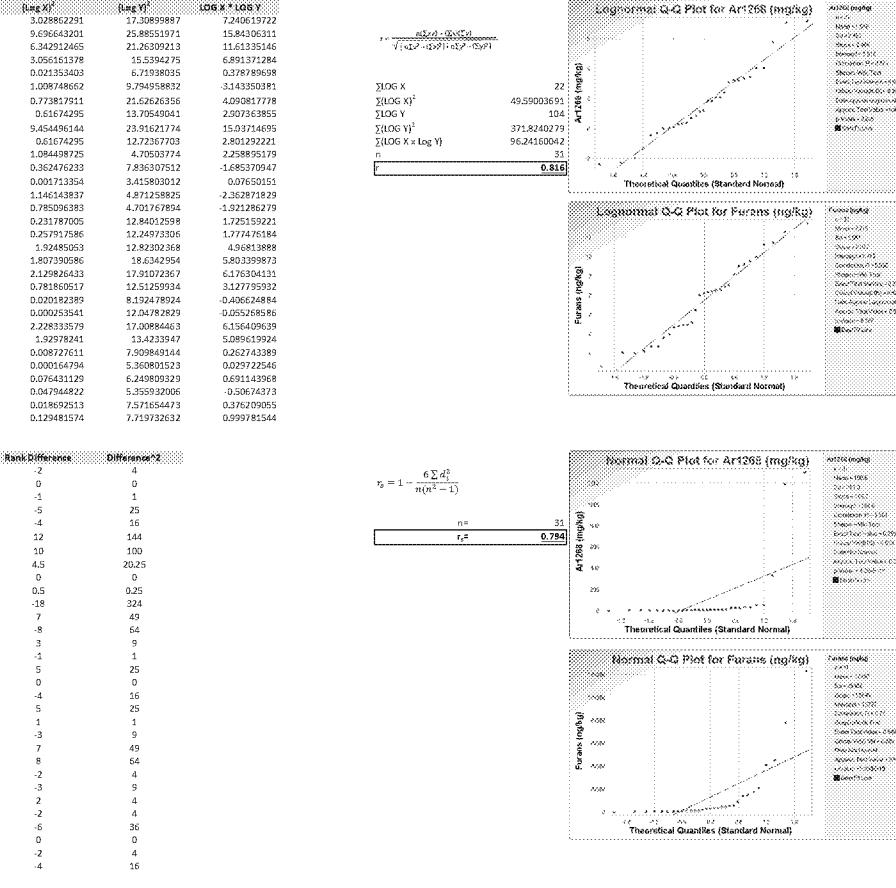
	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	4896.302435	1517.898675	3.255264426	0.0216193616	914.3523285	8819.44568	914.3523285	8819.44568
Ar1268 (mg/kg)	7854899847	9595625794	13.20021218	8.64297E-14	90.71939678	66.37860016	90.71939678	66.37860016

Pearson Correlation Analysis

Location	Log X	Log Y	(Log X)	(Log Y)	(Log X * Log Y)
36	1.7	4.2	3.028622931	17.30899887	7.240619722
61	3.1	5.1	9.696432021	25.885513971	15.84306311
68	2.5	4.6	6.342912465	21.263092123	11.61335146
1718	1.7	3.9	3.056151379	15.5394275	6.891371284
BR048	0.1	2.6	0.021354203	6.719380395	0.378789698
C-15	-1.0	3.1	1.009748662	9.794588582	-3.14330391
C-6	0.9	4.7	0.773817911	21.62626356	4.09817778
111	0.8	3.7	0.61576295	13.70549041	2.907363855
EPA-F2	3.1	4.9	9.454496144	23.91621774	15.03714695
GRID MARSH	0.8	3.6	0.61576295	12.72367703	2.801292221
117	1.0	2.2	1.084498725	4.70503774	2.258895179
110	-0.6	2.8	0.362476233	7.836307512	-1.685370947
100	0.0	1.8	0.001713354	3.415803012	0.07650151
101	-1.1	2.2	1.146143837	4.871258825	-2.352817829
102	-0.9	2.2	0.785096383	4.701767854	-1.921286279
D2-1A	0.5	3.6	0.2313787005	12.84092598	1.725159221
D2-1B	0.5	3.5	0.257917295	12.84092598	1.77443889
EC-3A	1.4	3.5	1.34930553	12.92402558	4.08615889
EC-3B	1.3	4.3	1.307390696	18.63423854	5.803339973
EC-4A	1.5	4.2	2.129362433	17.910726267	6.176304433
EC-4B	0.9	3.5	0.781860513	13.513593234	2.137719522
LC-1A	0.1	2.9	0.020392389	8.132478924	-0.406624884
LC-1B	0.0	3.5	0.002055841	12.04782829	-0.055288586
PC-1A	1.5	4.1	2.2283333579	17.00884463	6.156409639
PC-1B	1.4	3.7	1.92798241	13.42333547	5.096119924
PC-2A	0.1	2.8	0.008727611	7.509849144	0.262743389
PC-2B	0.0	2.3	0.000164794	5.3606001523	0.029722546
PC-3A	0.3	2.5	0.076431129	6.249809329	0.691143968
PC-3B	-0.2	2.3	0.04794482	5.559532006	-0.506747373
D1-2A	0.1	2.8	0.018692513	7.71654473	0.376209093
D1-2B	0.4	2.8	0.129481574	7.719732632	0.999781544

Spearman Correlation Analysis

Location	Aroclor 1268 Rank	Furan Rank	Rank Difference	Difference %
36	7	7	-2	4
61	1	0	0	0
68	3	4	-1	1
1718	4	0	5	25
BR048	20	24	-4	16
C-15	30	18	12	144
C-6	13	3	10	100
111	14.5	10	4.5	202.5
EPA-F2	2	2	0	0
GRID MARSH	14.5	14	0.5	0.25
117	11	29	-18	324
110	28	21	7	49
100	23	31	-8	54
101	31	28	3	9
102	29	30	-1	1
D2-1A	17	12	5	25
D2-1B	16	16	0	0
EC-3A	9	13	-4	16
EC-3B	10	5	5	25
EC-4A	7	6	1	1
EC-4B	12	15	-3	9
LC-1A	26	19	7	49
LC-1B	25	17	8	54
PC-1A	6	8	-2	4
PC-1B	8	11	-3	9
PC-2A	22	20	2	4
PC-2B	24	26	-2	4
PC-3A	19	25	-6	36
PC-3B	27	27	0	0
D1-2A	21	23	-2	4
D1-2B	18	22	-4	16



**APPENDIX E**

**Calculation for 95% UCL (ProUCL Input and Output)**

## PCDD/F TEQ in OU1 Sediment

### Notes:

\*TEQ results in ng/kg

Location	Parameter	val	D_val
D1-1A	TEQ	42.0	1
D1-1B	TEQ	51.5	1
D1-2A	TEQ	26.9	1
D1-2B	TEQ	27.6	1
D2-1A	TEQ	118.7	1
D2-1B	TEQ	71.0	1
EC-1A	TEQ	39.9	1
EC-1B	TEQ	39.3	1
EC-2A	TEQ	80.8	1
EC-2B	TEQ	14.1	1
EC-3A	TEQ	135.0	1
EC-3B	TEQ	863.3	1
EC-4A	TEQ	735.6	1
EC-4B	TEQ	123.9	1
LC-1A	TEQ	23.3	1
LC-1B	TEQ	112.4	1
MC-1A	TEQ	68.0	1
MC-1B	TEQ	50.4	1
MC-2A	TEQ	53.2	1
MC-2B	TEQ	69.2	1
MC-3A	TEQ	41.4	1
MC-3B	TEQ	56.1	1
PC-1A	TEQ	381.0	1
PC-1B	TEQ	121.3	1
PC-2A	TEQ	19.8	1
PC-2B	TEQ	11.6	1
PC-3A	TEQ	11.0	1
PC-3B	TEQ	6.9	1

### UCL Statistics for Data Sets with Non-Detects

#### User Selected Options

Date/Time of Computation ProUCL 5.17/13/2018 11:27:53 PM

From File Book1.xls

Full Precision OFF

Confidence Coefficient 95%

Number of Bootstrap Operations 2000

val

#### General Statistics

Total Number of Observations	28	Number of Distinct Observations	28
		Number of Missing Observations	0
Minimum	6.9	Mean	121.3
Maximum	863.3	Median	52.35
SD	205.2	Std. Error of Mean	38.77
Coefficient of Variation	1.692	Skewness	2.979

**Normal GOF Test**

Shapiro Wilk Test Statistic	0.526	<b>Shapiro Wilk GOF Test</b>
5% Shapiro Wilk Critical Value	0.924	Data Not Normal at 5% Significance Level
Lilliefors Test Statistic	0.366	<b>Lilliefors GOF Test</b>
5% Lilliefors Critical Value	0.164	Data Not Normal at 5% Significance Level
		Data Not Normal at 5% Significance Level

**Assuming Normal Distribution**

95% Normal UCL	95% UCLs (Adjusted for Skewness)		
95% Student's-t UCL	187.3	95% Adjusted-CLT UCL (Chen-1995)	208.4
		95% Modified-t UCL (Johnson-1978)	190.9

**Gamma GOF Test**

A-D Test Statistic	1.696	<b>Anderson-Darling Gamma GOF Test</b>
5% A-D Critical Value	0.783	Data Not Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.211	<b>Kolmogorov-Smirnov Gamma GOF Test</b>
5% K-S Critical Value	0.172	Data Not Gamma Distributed at 5% Significance Level
		Data Not Gamma Distributed at 5% Significance Level

**Gamma Statistics**

k hat (MLE)	0.791	k star (bias corrected MLE)	0.73
Theta hat (MLE)	153.4	Theta star (bias corrected MLE)	166.2
nu hat (MLE)	44.27	nu star (bias corrected)	40.86
MLE Mean (bias corrected)	121.3	MLE Sd (bias corrected)	142
Adjusted Level of Significance	0.0404	Approximate Chi Square Value (0.05)	27.21
		Adjusted Chi Square Value	26.52

**Assuming Gamma Distribution**

95% Approximate Gamma UCL (use when n>=50)	182.1	95% Adjusted Gamma UCL (use when n<50)	186.8
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**Lognormal GOF Test**

Shapiro Wilk Test Statistic	0.955	<b>Shapiro Wilk Lognormal GOF Test</b>
5% Shapiro Wilk Critical Value	0.924	Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.121	<b>Lilliefors Lognormal GOF Test</b>
5% Lilliefors Critical Value	0.164	Data appear Lognormal at 5% Significance Level
		Data appear Lognormal at 5% Significance Level

**Lognormal Statistics**

Minimum of Logged Data	1.932	Mean of logged Data	4.046
Maximum of Logged Data	6.761	SD of logged Data	1.152

**Assuming Lognormal Distribution**

95% H-UCL	199.7	90% Chebyshev (MVUE) UCL	189.3
95% Chebyshev (MVUE) UCL	226.7	97.5% Chebyshev (MVUE) UCL	278.4
99% Chebyshev (MVUE) UCL	380.1		

**Nonparametric Distribution Free UCL Statistics**

Data appear to follow a Discernible Distribution at 5% Significance Level

**Nonparametric Distribution Free UCLs**

95% CLT UCL	185	95% Jackknife UCL	187.3
95% Standard Bootstrap UCL	183	95% Bootstrap-t UCL	306.2
95% Hall's Bootstrap UCL	389.2	95% Percentile Bootstrap UCL	189.5
95% BCA Bootstrap UCL	208.9		
90% Chebyshev(Mean, Sd) UCL	237.6	95% Chebyshev(Mean, Sd) UCL	290.3
97.5% Chebyshev(Mean, Sd) UCL	363.4	99% Chebyshev(Mean, Sd) UCL	507

**Suggested UCL to Use**

95% H-UCL 199.7

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

Recommendations are based upon data size, data distribution, and skewness.

These recommendations are based upon the results of the simulation studies summarized in Singh, Maichle, and Lee (2006). However, simulations results will not cover all Real World data sets; for additional insight the user may want to consult a statistician.

ProUCL computes and outputs H-statistic based UCLs for historical reasons only.

H-statistic often results in unstable (both high and low) values of UCL95 as shown in examples in the Technical Guide.

It is therefore recommended to avoid the use of H-statistic based 95% UCLs.

Use of nonparametric methods are preferred to compute UCL95 for skewed data sets which do not follow a gamma distribution.